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SINGULAR BEHAVIOR OF THE LAPLACE OPERATOR IN POLAR SPHERICAL COORDINATES AND SOME OF ITS CONSEQUENCES FOR THE RADIAL WAVE FUNCTION AT THE ORIGIN OF COORDINATES

A. A. Khelashvili [a, b, 1], *T. P. Nadareishvili* [a, c, 2]

[a] Institute of High Energy Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi

[b] St. Andrea the First-Called Georgian University of Patriarchy of Georgia, Tbilisi

[c] Iv. Javakhishvili Tbilisi State University, Faculty of Exact and Natural Sciences, Tbilisi

Singular behavior of the Laplace operator in spherical coordinates is investigated. It is shown that in course of transition to the reduced radial wave function in the Schrödinger equation there appears additional term including the Dirac delta function, which was unnoted during the full history of physics and mathematics. The possibility of avoiding this contribution from the reduced radial equation is discussed. It is demonstrated that for this aim the necessary and sufficient condition is the requirement of the fast enough falling of the wave function at the origin. The result does not depend on character of potential — whether it is regular or singular. The various manifestations and consequences of this observation are considered as well. The cornerstone in our approach is the natural requirement that the solution of the radial equation at the same time must obey the full equation.

В работе исследуется сингулярное поведение оператора Лапласа в сферических координатах. Показано, что в процессе перехода к приведенной радиальной волновой функции в уравнении Шредингера появляется дополнительное слагаемое, которое содержит дельта-функцию Дирака, что оставалось незамеченным на протяжении всей истории физики и математики. Обсуждается возможность исключения этого вклада в расчеты с приведенным радиальным уравнением. Показано, что необходимым и достаточным условием для этого является требование достаточно быстрого спадания волновой функции в нуле. Результат не зависит от характера потенциала — является ли он гладкой или сингулярной функцией. Также демонстрируются различные эффекты и следствия исследуемого поведения. Краеугольным камнем представленного подхода является естественное требование, что решение радиального уравнения должно одновременно являться и решением полного уравнения.

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[1] E-mail: anzorkhelashvili@homail.com
[2] E-mail: teimuraz.nadareishvili@tsu.ge

INTRODUCTION

The aim of this paper is to survey the singular behavior of the Laplacian in spherical coordinates. Laplacian is encountered almost in all disciplines of theoretical physics as well as in mathematical physics. In this article, our attention is paid mostly to the Schrödinger equation, which in the Cartesian coordinates has the form (in units $\hbar = c = 1$):

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

where

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

is a Laplacian.

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

$$\psi(\mathbf{r}) = R(r)\,Y_l^m(\theta,\varphi) = \frac{u(r)}{r}\,Y_l^m(\theta,\varphi). \tag{3}$$

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

$$-\frac{1}{2m}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right]R(r) + \frac{l(l+1)}{2mr^2}\,R(r) + V(r)\,R(r) = ER(r) \tag{4}$$

or

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} + V(r)\right]u(r) = Eu(r). \tag{5}$$

All of this is well known from the classical textbooks on quantum mechanics, electrodynamics, etc. We display them here for further practical purposes. It will be shown below that the status of Eq. (5) is problematic.

From both mathematical and physical points of view, it is very important that the solutions of radial equations were compatible with the full Schrödinger equation (1). This is verbally mentioned in books, not only earlier [1, 2], but also in the modern ones [3]. For example, Dirac [1] wrote: *"Our equations ... strictly speaking, are not correct, but the error is restricted by only one point $r = 0$. It 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 about this problem (singularity of the Laplacian) for a long time, but character of singularity has never been specified. It was always underlined in mathematics that $r > 0$ strictly, but $r = 0$ is not somehow prominent point for the three-dimensional equation. Therefore, refinement of the behavior of the radial wave function at that point has a basic meaning in our opinion.

The first papers [4–7] on this problem appeared recently almost in parallel.

Because of relative novelty of this subject, below we will take some attention to its substantiation.

To complete the picture, we first discuss briefly the essence of this problem, and then some of its application will be considered.

In the teaching books and scientific articles two methods were applied in the transition from Eq. (4) to Eq. (5):

1. Substitution

$$R(r) = \frac{u(r)}{r} \tag{6}$$

into Eq. (4) or

2. Replacement of the differential expression in the parenthesis of Eq. (4) as [8–10] [1]:

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right] \to \frac{1}{r}\frac{d^2}{dr^2}(r). \tag{7}$$

We demonstrate below that in both cases the mistakes were made.

As all the principal information is concentrated in the Laplace operator, we begin with consideration of the classical Laplace equation in the vacuum (electrostatic equation).

1. THE LAPLACE EQUATION

Let us consider the Laplace equation in vacuum

$$\nabla^2\varphi(\mathbf{r}) = 0, \tag{8}$$

which in the Cartesian coordinates has the form

$$\nabla^2\varphi(\mathbf{r}) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\varphi(x, y, z) = 0. \tag{9}$$

This equation may be solved simply by separation of variables. The solution has the form [10]:

$$\varphi(x, y, z) = \mathrm{e}^{\pm i\alpha x}\,\mathrm{e}^{\pm i\beta y}\,\mathrm{e}^{\pm\sqrt{\alpha^2+\beta^2}z}. \tag{10}$$

Clearly the solution is regular everywhere and at the origin is constant

$$\varphi(0) = \mathrm{const}. \tag{11}$$

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

Now, let us find the spherically symmetric solution. The corresponding equation is written as [8]:

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\varphi(r) = 0. \tag{12}$$

Certainly, it was possible passing to spherical coordinates in Eq. (9), substituting (3) and taking zero angular momentum. We will arrive again to Eq. (12).

[1] In the fundamental book of J. D. Jackson [10], this relation is even exhibited on the cover-page in the list of the most fundamental forms!

The operator in parenthesis of Eq. (12) is often rewritten ([8], Ch. 20, [9], etc.) according to (7), and subsequently, Eq. (12) takes the form

$$\frac{1}{r}\frac{d^2}{dr^2}(r\varphi) = 0, \tag{13}$$

the solution of which is

$$u(r) \equiv r\varphi = ar + b. \tag{14}$$

But, determining from here the function

$$\varphi = a + \frac{b}{r} \tag{15}$$

does not obey Eq. (12), because

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right) = -4\pi\delta^{(3)}(\mathbf{r}), \tag{16}$$

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

What happens? *It seems that we made an illegal action somewhere* (see, Feynman [8]).

It is possible to consider this problem by another way also, namely, following the substitution (6), take

$$\varphi(r) = \frac{u(r)}{r} \tag{17}$$

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

$$\frac{1}{r}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) u(r) + u(r)\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right) + 2\frac{du}{dr}\frac{d}{dr}\left(\frac{1}{r}\right) = 0. \tag{18}$$

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

$$\frac{1}{r}\frac{d^2u}{dr^2} + u\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right) = 0, \tag{19}$$

but, according to Eq. (16), instead of Eq. (13), it follows

$$\frac{1}{r}\frac{d^2u}{dr^2} - 4\pi\delta^{(3)}(\mathbf{r})\, u(r) = 0. \tag{20}$$

The appearance of the delta function here is unexpected. Comparing this one with Eq. (13), we conclude that the representation of the Laplace operator in the form (7) is not valid *everywhere*. The correct form is [5, 7]:

$$\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} = \frac{1}{r}\frac{d^2}{dr^2}(r\cdot) - 4\pi\delta^{(3)}(\mathbf{r})r\cdot. \tag{21}$$

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

It is evident, that after substitutions

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\varphi \Rightarrow \frac{1}{r}\frac{d^2}{dr^2}(r\varphi) \quad \text{and} \quad u=r\varphi, \tag{22}$$

the solution $\varphi = u/r$, obtained from Eq. (13), never satisfies the initial equation (12) *everywhere*.

By unknown for us reasons, this simple fact stayed unnoted till now and in all papers as well as in all books the expression (7) was used. As we made clear above, in this case, the obtained solution (15) looks like if there is a point source at the origin. However, it is not so — mathematical reason is that in spherical coordinates the point $r = 0$ is absent. The Jacobian of transformation to spherical coordinates has the form $J = r^2 \sin\theta$ and is singular at points $r = 0$ and $\theta = n\pi\,(n = 0, 1, 2, \ldots)$.

Singularity in angles is eliminated by requirements of continuity and uniqueness, which lead to spherical harmonics $Y_l^m(\theta, \varphi)$. As regards of the radial variable r, there is no such a restriction for it. Therefore, if we want to derive the solution valid everywhere, we are forced to take the delta function into consideration.

It must be noted that the appearance of the delta function in the Laplace equation was discussed also in article [6], where the difference between spaces R^n and $R^n/\{0\}$ is studied from the positions of distribution theory.

The question is: *how to formulate the problem in such a way that to retain all results derived earlier for the central potentials with the aid of traditional reduced radial equation* (5) *containing the second derivative only?* One of the reasonable ways is the following: as in spherical coordinates $\delta^{(3)}(\mathbf{r}) = \dfrac{\delta(r)}{4\pi r^2}$ [11], Eq. (20) can be reduced to

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

or

$$r\frac{d^2u}{dr^2} - u(0)\delta(r) = 0. \tag{24}$$

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

$$u(0) = 0. \tag{25}$$

Moreover, the delta function is "overcome" if at least

$$\lim_{r\to 0} u(r) \approx r. \tag{26}$$

Then, owing to the relation $r\delta(r) = 0$, the extra term falls out and the standard equation (13) follows. Let us look first what the condition (25) gives in the above-considered solution (14). Requiring (25), it follows $b = 0$, i.e., $u = ar$ and $\varphi(r) = a = \text{const}$. Hence, we obtain the correct, consisting with the full equation (8), value (11). It is consisting also with the real physical picture.

Therefore, in the reduced radial equation (5) we must consider only such a class of solutions, which vanish at the origin. The other entire boundary conditions lose the physical meaning and have only mathematical interest. It is precisely the main result of this section — Eq. (5) gives the consistent with the primary equation in Cartesian coordinate's solution only if the restriction (25) is satisfied. Appearance of this condition is purely geometrical (not a dynamical) artefact. In short, Eq. (5) and the condition (25) appear simultaneously.

2. THE RADIAL SCHRÖDINGER EQUATION AND $u(0)$

As an example, let us consider the radial Schrödinger equation (4).

After the substitution (6), according to the above-mentioned about the Laplace operator, we obtain the following form of this equation:

$$\frac{1}{r}\left[\frac{d^2u(r)}{dr^2}-\frac{l(l+1)}{r^2}u(r)\right]-\frac{\delta(r)}{r^2}u(r)+2m\left[E-V(r)\right]\frac{u(r)}{r}=0. \tag{27}$$

To single out the true singularity, let us multiply this equation on r^2 and integrate by dr in a sphere of small radius a. We derive

$$\int\limits_0^a r\frac{d^2u(r)}{dr^2}\,dr-l(l+1)\int\limits_0^a\frac{u(r)}{r}dr-u(0)+\int\limits_0^a\left(2mE-V(r)\right)\,u(r)r\,dr=0. \tag{28}$$

From here we determine

$$u(0)=\int\limits_0^a r\frac{d^2u(r)}{dr^2}\,dr-l(l+1)\int\limits_0^a\frac{u(r)}{r}dr+\int\limits_0^a\left(2mE-V(r)\right)\,u(r)r\,dr. \tag{29}$$

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

$$\underset{r\to0}{u(r)}\approx r^s \tag{30}$$

and the potential as

$$\underset{r\to0}{V(r)}\approx\frac{g}{r^n},\quad n>0. \tag{31}$$

Then, the integration in Eq. (29) may be easily performed and we obtain

$$u(0)=\left[\frac{s(s-1)-l(l+1)}{s}r^s+\frac{2mE}{s+2}\,r^{s+2}-\frac{2mg}{s+2-n}\,r^{s+2-n}\right]_0^a. \tag{32}$$

We must remove the extra delta term from Eq. (27), because, otherwise, we do not get the usual form of radial equation (5).

If we retain $u(0)$ in Eq. (28), then there are three possible values for it: $u(0)=0$, $u(0)$ is finite, and $u(0)=\infty$. Note, that all the enumerated values do not contradict the normalization condition near the origin $\int\limits_0^a u^2\,dr<\infty$, but not all of them are useful.

The first value is preferable among them, because in opposite cases — finite $u(0)$ will give $R\approx\mathrm{const}/r$ at the origin and in Eq. (27) the delta function reappears. Therefore, this solution will not obey the full Schrödinger equation. The last value, $u(0)=\infty$ is, of course, unacceptable, because to have an infinite number in equation is senseless.

There remains only one reasonable value, Eq. (25). Moreover, this restriction takes place in spite of the potential is regular or singular. Singularity of the potential effects only the law of turning of $u(r)$ to zero. This follows from the relation (32) as all the exponents here must be positive. We will have therefore

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

It follows from the last inequality that when the index of singularity of potential n increases, the index of wave function behavior s must also increase. Moreover, we must have $s \geqslant 1$ in order the wave function at the origin "overcomes" the delta function in the term $u(r)\,\delta(r)$. Therefore, there remain the final allowed inequalities

$$s \geqslant 1, \quad s + 2 - n > 0. \tag{33}$$

If, in addition, we require this production to be a distribution, it becomes necessary $u(r)$ to be an infinitely smooth function [12, 13], i.e., in Eq. (30) we must have $s \geqslant 1$ and the index s is an integer number.

Thus, the wave function must be the sufficiently regular one at the origin. This fact may have far-reaching consequences.

3. SOME APPLICATIONS

The first question, that appears here, is the following: under what conditions can we maintain the standard form of reduced wave equation?

Basing on the previous considerations, we suppose that the equation in the standard form (5) takes place and clarify for which potentials it happens, i.e., when can we satisfy the restriction (25)?

3.1. Regular Potentials. Let us consider first the regular potentials

$$\lim_{r\to 0} r^2 V(r) = 0. \tag{34}$$

Then, in the Schrödinger equation (5) the leading asymptotic at the origin is determined by a centrifugal term and the characteristic equation takes the form $s(s-1) = l(l+1)$. So,

$$\underset{r\to 0}{u} \sim c_1 r^{l+1} + c_2 r^{-l}, \quad l = 0, 1, 2 \ldots \tag{35}$$

We must retain only the first solution, because now $s = l + 1 \geqslant 1$, and the derived representation is satisfied (s is an integer number!). At the same time, the second solution with $s = -l$ must be ignored even for $l = 0$ [14]. The second solution does not satisfy the three-dimensional Schrödinger equation (1), as after its substitution the Laplacian produces l-fold derivatives of delta function [14].

Resuming the above-said, we conclude that in case of regular potentials (34) the radial equation (5) remains, because, in this case, all the requirements are realized and, consequently, the results obtained earlier by this equation remain valid without any changes!

3.2. Weakly-Singular Transitive Potentials. Let us now consider potentials that are intermediate between singular and regular ones, the so-called weakly-singular potentials of the form

$$\lim_{r\to 0} r^2 V(r) = -V_0 = \text{const}. \tag{36}$$

Here $V_0 > 0$ corresponds to the attraction, while $V_0 < 0$ — to the repulsion. Now, the behavior of $u(r)$ at the origin is

$$\underset{r\to 0}{u} \sim d_1 r^{1/2+P} + d_2 r^{1/2-P}, \quad P = \sqrt{\left(l + \frac{1}{2}\right)^2 - 2mV_0} > 0. \tag{37}$$

In order that the usual equation (5) will still remain, according to Eq. (33), we must have $(s \geqslant 1)$, i.e., $P \geqslant 1/2$ for all l, including $l = 0$, and, at the same time, according to requirement of the distribution theory, $1/2 + P = N$, $N = 1, 2, 3 \ldots$ So, it results in a "strange quantization" of V_0, which is also senseless. It follows that, in this case, there are no solutions except for "quantized" V_0.

We see that the second solution in Eq. (37) must be discarded. Note, that in scientific literature there is no definite viewpoint concerning this (see, e.g., book by R. Newton [15] and various modern articles [16, 17]). Therefore, the above-mentioned derivation is the first correct one.

3.3. The Problem of Self-Adjoint Extention (SAE). Last decades the problem of self-adjoint extension (SAE) of radial Hamiltonian

$$H_r \equiv -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + 2mV(r) \tag{38}$$

was often considered in cases of singular potentials, like the above one. In this problem the essential role plays the behavior of radial wave functions $u(r)$ at the origin of coordinates. For example, the condition of self-adjointicity of Hamiltonian (38) has the form [18]:

$$\int_0^\infty u_1 \hat{H}_r u_2 \, dr - \int_0^\infty u_2 \hat{H}_r u_1 \, dr = \frac{1}{2} \lim_{r \to 0} [u_2(r) u_1'(r) - u_1(r) u_2'(r)] = 0, \tag{39}$$

where $u_{1,2}(r) \equiv rR_{1,2}(r)$ are two linearly independent solutions of the reduced radial equation (5) corresponding to different eigenvalues of the Hamiltonian (38). There were considered various boundary conditions such as the ones of Dirichlet, Neumann, and the most general condition of Robin [19]. *As we made clear above, only the Dirichlet condition (25) is right.*

In most articles in course of discussion of SAE procedure with the Hamiltonian (38) the authors pay attention only to square integrability of the wave function [20]. But it is not sufficient in all cases. Still W. Pauli [21] noted that "the eigenfunction, for which $\lim\limits_{r \to 0}(rR) \neq 0$, is not permissible (even if $\int\limits_0^\infty R^* R r^2 \, dr$ exists for such functions)". The same is confirmed in the more modern books (for example, in [3, pf 52] the author says: "It can be shown that the condition $u(0) = 0$ follows from the requirement that the solution of the Schrödinger equation in spherical coordinates must be also solution when the equation is written in Cartesian coordinates"). But, unfortunately, this thesis is not shown regularly in this book, especially for singular potentials.

If we impose the boundary condition with the indices $s \geqslant 1$, we must restrict ourselves only by the first (regular) solution, i.e., $d_2 = 0$ (see, Eq. (37)). Then, the radial Hamiltonian (38) becomes a self-adjoint one automatically and the SAE is not needed. As for the first solution, the condition $P \geqslant 1/2$ is achieved only if

$$l(l+1) > 2mV_0, \tag{40}$$

i.e., for $l = 0$ only $V_0 < 0$ is permissible and as regards of other admissible values, from the condition $1/2 + P = N$ follows a strange "quantization" of V_0:

$$V_0 = \frac{(l+1/2)^2 - (N-1/2)^2}{2m}, \quad N = 1, 2, 3 \ldots \tag{41}$$

Hence, even for such a simple singular potential (36) Eq. (5) meets the serious physical difficulties.

We do not consider here the other, more singular potentials, because the general tendency is obvious. The Hamiltonian (38) by itself is always self-adjoint on the regular solutions, satisfying (25), as it follows from the condition (39) and restrictions (33) for any singular potentials. For all other boundary conditions the Hamiltonian (38) will not bear a relation to physics, because this form of Hamiltonian emerges only together with condition (25).

We conclude that the reduced radial equation (5) may be applied for all regular potentials, nevertheless for singular potentials one must work only with the total radial equation (4) and, consequently, use the full radial Hamiltonian

$$H_R = -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2} + 2mV(r), \tag{42}$$

but search for regular solutions only. In [4], we have shown that from the finiteness of the differential probability $dW = |R(r)|^2 r^2\, dr$ and the time independence of the norm, it follows that $R(r)$ is less singular at the origin than $1/r$, or

$$\lim_{r\to 0} rR = 0, \tag{43}$$

which is evidently consistent with $u(0) = 0$.

Moreover, in case of fulfillment of this condition, the radial equation (4) for full radial function $R(r)$ is equivalent to the Schrödinger equation (1). This equivalence takes place only in nonsingular solutions. In other words, Eq. (4) is equivalent to the three-dimensional Schrödinger equation only for regular solutions. This was proved also in [6] in the framework of the distribution theory.

For demonstration of principal difference between the full and reduced radial Hamiltonians let us consider now the same problem in view of the full radial function $R(r)$. The condition (43) is the only boundary restriction for it, which is not so severe. Therefore, there appears a possibility to retain the second solution as well in the case of singular potentials behaving like (36).

The following statement can be proved:

Theorem. The radial Schrödinger equation (4) except the standard (nonsingular) solutions has also additional solutions for attractive potentials, like (36), when the following condition is satisfied:

$$l(l+1) < 2mV_0. \tag{44}$$

The proof of this theorem is straightforward.

Indeed, for the attractive potential (36) *at small distances* this equation reduces to

$$R'' + \frac{2}{r}R' - \frac{P^2 - 1/4}{r^2}R = 0, \tag{45}$$

where P is defined by (37).

Therefore, Eq. (45) has the following solution:

$$\lim_{r\to 0} R = a_{\mathrm{st}}\, r^{-1/2+P} + a_{\mathrm{add}}\, r^{-1/2-P} \equiv R_{\mathrm{st}} + R_{\mathrm{add}}. \tag{46}$$

So, we have two regions for this parameter P. In the interval

$$0 < P < 1/2 \tag{47}$$

the second term $a_{\rm add}\, r^{-1/2-P} = R_{\rm add}$ must also be retained, because the boundary condition (43) is fulfilled for it. The potential like (36) was first considered by K. Case [22], but he ignored the second term in solution. As regards of a region $P \geqslant 1/2$, only the first term $a_{\rm st}\, r^{-1/2+P} = R_{\rm st}$ must be retained.

From Eqs. (37) and (47) follows the condition (44) for existence of additional states. If we demand the reality of P (otherwise, "falling" to centre takes place [22–24]), the parameter V_0 would be restricted by the condition

$$2mV_0 < l(l+1) + \frac{1}{4}. \tag{48}$$

The last two inequalities restrict $2mV_0$ in the following interval:

$$l(l+1) < 2mV_0 < l(l+1) + \frac{1}{4}. \tag{49}$$

Intervals from the left and from the right sides have no crossing and therefore, if additional solution exists for fixed V_0 and for some l, then it is absent for another l.

Thus, we see from (44) that in the $l = 0$ state, except the standard solutions, there are additional solutions too for arbitrary small V_0, while for $l \neq 0$ the "strong" field is required in order to fulfil (44).

As the additional solutions obey all physical requirements in the interval (47), one has to retain this solution as well and study its consequences.

For definiteness consider the potential

$$V = -\frac{V_0}{r^2}, \quad V_0 > 0. \tag{50}$$

When $E = 0$, the solution of the full radial equation (4) has the form in whole space

$$R = Ar^{-1/2+P} + Br^{-1/2-P}. \tag{51}$$

There is only one worthy case, namely, $0 < P < 1/2$. We see that the wave function has a simple zero, determined by

$$r = r_0 = \left(-\frac{B}{A}\right)^{1/P}. \tag{52}$$

(It is evident from this relation that constants A and B must have opposite signs in order for r_0 to be real number.) Hence, the wave function has only one node and according to the well-known theorem (*the number of bound states coincides with the number of nodes of radial wave function $R(r)$ in $E = 0$ state* [2]), we have exactly one bound state.

This result differs from that considered in any textbooks on quantum mechanics.

We can give very simple physical picture of how the additional solutions arise. For this purpose, let us rewrite the Schrödinger equation near the origin for attractive potential (36) in the form

$$R'' + \frac{2}{r}R' + 2m\left[E - V_{\rm ac}(r)\right]R = 0, \tag{53}$$

where

$$V_{\rm ac} = \frac{P^2 - 1/4}{2mr^2}. \tag{54}$$

Consider the following possible cases:

i) If $P > 1/2$, then $V_{\rm ac} > 0$ and it is repulsive centrifugal potential and as we saw, one has no additional solutions.

ii) If $0 < P < 1/2$, then $V_{\rm ac} < 0$. Therefore, it becomes attractive and is called as quantum anticentrifugal potential [25]. This potential has $R_{\rm add}$ states, because the condition (43) is fulfilled in this case.

iii) If $P^2 < 0$, then $V_{\rm ac}$ becomes strongly attractive and one has "falling to the center".

Therefore, the sign of the potential $V_{\rm ac}$ determines whether we need additional solutions or not.

3.4. SAE Procedure for Full Radial Hamiltonian in "Pragmatic" Approach. Considering some consequences from the point of the above-mentioned results, let us first of all remember some issues of SAE procedure.

If for any functions u and v, given operator $\hat{A}$ satisfies the condition

$$\langle v \,|\, \hat{A}u\rangle = \langle \hat{A}v \,|\, u\rangle, \tag{55}$$

then this operator is called Hermitian (or symmetric). For self-adjointness it is required in addition that the domains of functions of operators $\hat{A}$ and $\hat{A}^+$ would be equal. As a rule, the domain of $\hat{A}^+$ is wider and it becomes necessary to make a self-adjoint extension of the operator $\hat{A}$.

There exists a well-known powerful mathematical apparatus for this purpose [26, 27].

It may happen that the operator is Hermitian, but its self-adjoint extension is impossible, i.e., Hermiticity is the *necessary, but not sufficient condition* for self-adjointness. Good example is the operator of the radial momentum p_r, which is Hermitian on functions that satisfy the condition (43), but its extension to the self-adjoint one is impossible (see, L. D. Faddeev's remark in the A. Messiah's book — Russian translation, footnote in p. 336 [28]).

Our subject of interest is the radial Hamiltonian (42) and, consequently, Eq. (4).

It is easy to see that for any two eigenfunctions R_1 and R_2 corresponding to the levels E_1 and E_2 of the radial Hamiltonian $\hat{H}_R$, the condition (55) takes the following form:

$$\int\limits_0^\infty R_1 \hat{H}_R R_2 r^2\, dr - \int\limits_0^\infty R_2 \hat{H}_R R_1 r^2\, dr = 2m\,(E_2 - E_1) \int\limits_0^\infty R_1 R_2 r^2\, dr. \tag{56}$$

It follows that a self-adjoint condition is proportional to the orthogonality integral, therefore these two conditions are mutually dependent. As the self-adjoint operator has orthogonal eigenfunctions, requirement of orthogonality automatically provides self-adjointness of H_R, which means that this way provides realization of SAE procedure. It is an essence of the so-called "pragmatic approach" [29], which is much simpler and gets the same results as the strong mathematical full SAE procedure, provided the fundamental condition (43) is not violated. Moreover, this method is physically more transparent. Just this method had been used by K. Case in his well-known paper [22], but he did consider only the regular solution.

Notice that all above considerations are true only for the radial Hamiltonian operator $\hat{H}_R$, because for other operators proportionality like (56) does not arise.

3.5. Explicit Solution of the Schrödinger Equation for the Inverse Squared Potential. It was thought that potential (50) has no levels out of the region of "falling to the center" (see, e.g., [22, 23]), but in [16, 20, 30] single level was found by complete SAE procedure, while the boundary condition and the range of parameter like P are questionable there. Here we will show explicitly that this potential has exactly single level, which depends on the SAE parameter τ.

Let us now study in which cases the right-hand side of (56) is vanishing. We must distinguish regular and transitive potentials. As we are interested in bound states, we suppose that the full radial function decreases sufficiently fast at infinity. So, the behavior at the origin is relevant for our aims.

In case of regular potentials (34), as was mentioned above, we retain only first, regular (or standard) solution at the origin

$$\underset{r\to 0}{R_{\rm st}} \sim a_{\rm st} r^{\,l+1}. \tag{57}$$

Calculating the right-hand side of (56) by this function, we get zero. Therefore, for regular potentials the radial Hamiltonian $\hat{H}_R$ is self-adjoint on regular solutions and does not need SAE.

Contrary to this case, for transitive attractive (36) potential one has to retain the additional solution $\underset{r\to 0}{R_{\rm add}} \sim r^{-1/2-P}$ as well, because there are no reasons to neglect it. Now, for both solutions, the right-hand sides of (56) are not zero in general. Indeed, they equal to

$$m(E_1 - E_2) \int\limits_0^\infty R_2 R_1 r^2\, dr = P\left(a_1^{\rm st} a_2^{\rm add} - a_2^{\rm st} a_1^{\rm add}\right). \tag{58}$$

Remark. The case $P = 0$ must be considered separately, when the general solution of (4) behaves as

$$\lim_{r\to 0} R = a_{\rm st}\, r^{-1/2} + a_{\rm add}\, r^{-1/2} \ln r = R_{\rm st} + R_{\rm add}. \tag{59}$$

So, instead of (58) one obtains

$$m(E_1 - E_2) \int\limits_0^\infty R_2 R_1 r^2\, dr = -\frac{1}{2}\left(a_1^{\rm st} a_2^{\rm add} - a_2^{\rm st} a_1^{\rm add}\right). \tag{60}$$

Thus, retaining additional solution causes the breakdown of orthogonality condition and, consequently, $\hat{H}_R$ is no more a self-adjoint operator.

It is natural to ask — how to fulfil the orthogonality condition? It is clear, that in both $P \neq 0$ and $P = 0$ cases, one must require

$$a_1^{\rm st} a_2^{\rm add} - a_2^{\rm st} a_1^{\rm add} = 0 \tag{61}$$

or equivalently

$$\frac{a_{1\rm add}}{a_{1\rm st}} = \frac{a_{2\rm add}}{a_{2\rm st}}. \tag{62}$$

In this case, the radial Hamiltonian $\hat{H}_R$ becomes a self-adjoint operator. This generalizes the Case result [22], who considered only standard solution.

So, it is necessary to introduce the so-called SAE parameter, which in our case may be defined as

$$\tau \equiv \frac{a_{\rm add}}{a_{\rm st}}, \tag{63}$$

τ parameter is the same for all levels (for fixed orbital l momentum) and is real for bound states.

Now, let us return to the solution of the Schrödinger equation for potential (50)

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(-k^2 - \frac{P^2 - 1/4}{r^2}\right) R = 0, \tag{64}$$

where P is given by (37) and

$$k^2 = -2mE > 0 \quad (E < 0). \tag{65}$$

One can reduce Eq. (64) to the equation for modified Bessel functions by substitutions

$$R(r) = \frac{f(r)}{\sqrt{r}}, \quad x = kr, \tag{66}$$

leading to the following equation:

$$x^2 \frac{d^2 f(x)}{dx^2} + x\frac{df(x)}{dx} - \left(x^2 + P^2\right) f(x) = 0. \tag{67}$$

This equation has three pairs of independent solutions: $I_P(kr)$ and $I_{-P}(kr)$, $I_P(kr)$ and $\mathrm{e}^{i\pi P}K_P(kr)$, $I_{-P}(kr)$ and $\mathrm{e}^{i\pi P}K_P(kr)$, where $I_P(kr)$ and $K_P(kr)$ are the Bessel and MacDonald modified functions, respectively [31].

Careful analysis gives that the relevant pair is the first one only, i.e., the pair $I_P(kr)$ and $I_{-P}(kr)$.

So, the general solution of (64) is

$$R = r^{-1/2}\left[AI_P(kr) + BI_{-P}(kr)\right]. \tag{68}$$

Consider the behavior of this solution at small and large distances:

a) In case of small distances (see, [31]),

$$\underset{z\to 0}{I_P(z)} \approx \left(\frac{z}{2}\right)^P \frac{1}{\Gamma(P+1)}. \tag{69}$$

Then, it follows from (68) and (69) that

$$\lim_{r\to 0} R(r) \approx r^{-1/2}\left[A\left(\frac{k}{2}\right)^P \frac{r^P}{\Gamma(P+1)} + B\left(\frac{k}{2}\right)^{-P} \frac{r^{-P}}{\Gamma(1-P)}\right]. \tag{70}$$

From (46), (62), (70) and the definition (63) we obtain

$$\tau = \frac{B}{A} 2^{2P} k^{-2P}. \tag{71}$$

b) At large distances, we have [31]:

$$I_P(z) \underset{z\to\infty}{\approx} \frac{\mathrm{e}^z}{\sqrt{2\pi z}} \tag{72}$$

and

$$R(r) \underset{r\to\infty}{\approx} \frac{1}{\sqrt{2\pi}}\{A+B\}\,\mathrm{e}^{kr}. \tag{73}$$

Therefore, requiring vanishing of $R(r)$ at infinity, we have to take

$$B = -A, \tag{74}$$

and from (71), (74) and (65) we obtain one real level (for fixed orbital l momentum, satisfying (44)),

$$E = -\frac{2}{m}\left[-\frac{1}{\tau}\right]^{1/P}, \quad 0 < P < 1/2. \tag{75}$$

Equation (75) is a new expression derived as a consequence of orthogonality condition in the framework of "pragmatic" approach.

Reality of energy in (75) restricts τ parameter to be negative $\tau < 0$. In general, τ is a free parameter, but some physical requirements may restrict its magnitude. Note, that this level is absent in standard quantum mechanics ($\tau = 0$) — it appears when one performs SAE procedure.

To obtain the corresponding wave function, take into account the well-known relation [31]:

$$K_P(z) = \frac{\pi}{2\sin\,P\pi}\left[I_{-P}(z) - I_P(z)\right]. \tag{76}$$

Then, the wave function corresponding to the level (75) is

$$R = -A\frac{2}{\pi}r^{-1/2}\sin\,P\pi K_P(kr). \tag{77}$$

Because of exponential damping

$$K_P(z) \underset{z\to\infty}{\approx} \sqrt{\frac{\pi}{2z}}\,\mathrm{e}^{-z}, \tag{78}$$

the function (77) corresponds to the bound state. It is also known that $K_P(z)$ function has no zeroes for real $P(0 < P < 1/2)$, and therefore (75) corresponds to a single bound state. Moreover, wave function (77) satisfies the fundamental condition (43) for $0 < P < 1/2$.

Let us make some comments.

a) In [20], it was noticed that single bound state may be observed experimentally in polar molecules. For example, H_2S and HCl atoms exhibit anomalous electron scattering [32,33], which can be explained only by electron capture. Indeed, for those molecules electron is moving in a point dipole field, and, in this case, the problem is reduced to the Schrödinger equation with a potential (50). Thus, a level (75) obtained theoretically may be observed in those experiments.

b) It was commonly believed, that the potential

$$V = -\frac{V_0}{sh^2\alpha r} \tag{79}$$

has no levels in region (47) (see, for example, problem 4.39 in [34]). In [34], by the arguments of the well-known comparison theorem [26], which in this case looks like

$$-\frac{V_0}{sh^2\alpha r} \geqslant -\frac{V_0}{\alpha^2 r^2}, \tag{80}$$

it is concluded that the potential (79) cannot have a level in the area (47), because the potential (50) has no levels in this area. But, as we know, there is τ-dependent one level (75), therefore the levels for (79) are expected. Indeed, in [35] by using the Nikiforov–Uvarov method [36], it was shown that the potential (79) has infinite number of levels in the region (47).

4. OTHER APPLICATIONS

There are physically more realistic potentials, which differ from (50), but behave as r^{-2} at the origin.

Famous examples are molecular potential (valence electron model), the Coulomb potential in the Klein–Gordon equation, etc.

4.1. Valence Electron Model. Let us consider a molecular potential, having the following form:

$$V = -\frac{V_0}{r^2} - \frac{\alpha}{r} \quad (V_0, \alpha > 0)\,. \tag{81}$$

Because of a singular r^{-2}-like behavior at the origin, one must consider equation for the $R(r)$ function, which in dimensionless variables takes the form

$$\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{P^2 - 1/4}{\rho^2} + \frac{\lambda}{\rho} - \frac{1}{4}\right) R = 0, \tag{82}$$

where

$$\rho = \sqrt{-8mE}\,r = ar, \quad \lambda = \frac{2m\alpha}{\sqrt{-8mE}} > 0, \quad E < 0, \tag{83}$$

and P is again given by Eq. (37).

If we substitute

$$R = \rho^{-1/2+P}\,\mathrm{e}^{-\rho/2} F(\rho), \tag{84}$$

the equation for confluent hypergeometric functions follows

$$\rho F'' + (2P + 1 - \rho)\,F' - (1/2 + P - \lambda)F = 0. \tag{85}$$

This equation has four independent solutions, two of which constitute a fundamental system of solutions [37]. They are (in notations of [37]):

$$\begin{aligned} &y_1 = F(a, b; \rho), \quad y_2 = \rho^{1-b} F(1 + a - b, 2 - b; \rho), \\ &y_5 = \Psi(a, b; \rho), \quad y_7 = \mathrm{e}^{\rho}\,\Psi(b - a, b; -\rho), \end{aligned} \tag{86}$$

where

$$a = 1/2 + P - \lambda, \quad b = 1 + 2P. \tag{87}$$

Only y_1 is considered in the scientific articles, as well as in all textbooks (see, e.g., [23, 38]). Requiring $a = -n \quad (n = 0, 1, 2 \ldots)$, the standard levels follow. Other solutions (y_2, y_5, y_7) have singular behavior at the origin and usually they are not taken into account. But the singularity in case of attractive potentials like (36) has the form $r^{-1/2-P}$ and in the region $0 < P < 1/2$ other solutions must be considered as well. Therefore, the problem becomes more "rich".

Let us consider a pair y_1 and y_2. The general solution of (85) is

$$R = C_1 \rho^{-1/2+P} \, \mathrm{e}^{-\rho/2} F\left(1/2 + P - \lambda, 1 + 2P; \rho\right) + \\ + C_2 \rho^{-1/2-P} \, \mathrm{e}^{-\rho/2} F(1/2 - P - \lambda, 1 - 2P; \rho). \tag{88}$$

Considering Eq. (88) at the origin and accounting Eq. (63), we obtain the following expression for SAE τ parameter:

$$\tau = \frac{C_2}{C_1} \frac{1}{(-8mE)^P}. \tag{89}$$

On the other hand, R must decrease at infinity. From the well-known asymptotic properties of confluent hypergeometric function F, we find the following restriction:

$$C_1 \frac{\Gamma(1 + 2P)}{\Gamma(1/2 + P - \lambda)} + C_2 \frac{\Gamma(1 - 2P)}{\Gamma(1/2 - P - \lambda)} = 0. \tag{90}$$

It gives the equation for eigenvalues in terms of τ parameter

$$\frac{\Gamma(1/2 - \lambda - P)}{\Gamma(1/2 - \lambda + P)} = -\tau(-8mE)^P \frac{\Gamma(1 - 2P)}{\Gamma(1 + 2P)}. \tag{91}$$

This is very complicated transcendental equation for E, depending on τ parameter. There are two values of τ, when this equation can be solved analytically:

i) $\tau = 0$. In this case, we have only standard levels, which can be found from the poles of $\Gamma(1/2 - \lambda + P)$:

$$1/2 - \lambda + P = -n_r, \quad n_r = 0, 1, 2 \ldots \tag{92}$$

ii) $\tau = \pm\infty$. In this case, we have only additional levels, obtained from the poles of $\Gamma(1/2 - \lambda - P)$:

$$1/2 - \lambda - P = -n_r, \quad n_r = 0, 1, 2 \ldots \tag{93}$$

Thus, in these cases, one can obtain explicit expressions for standard and additional levels

$$E_{\mathrm{st,add}} = -\frac{m\alpha^2}{2[1/2 + n_r \pm P]^2} = -\frac{m\alpha^2}{2[1/2 + n_r \pm \sqrt{(l + 1/2)^2 - 2mV_0}]^2}, \tag{94}$$

where signs $(+)$ or $(-)$ correspond to standard and additional levels, respectively.

We note that only Eq. (92) was known till now. So, Eq. (91) and its consequences are new results.

Notice also that, in case $V_0 < 0$, we obtain the well-known Kratzer potential [38], but now the condition (44) is not satisfied. Therefore, there are no additional levels for the Kratzer potential.

It is remarkable that the function (88) may be rewritten in unified form by using the following relation for the Whittaker functions [39]:

$$W_{a,b}(x) = \mathrm{e}^{-1/2x}\, x^{1/2+b} \frac{\pi}{\sin \pi(1+2b)} \times \\ \times \left[\frac{F\left(1/2+b-a,\ 1+2b;\ x\right)}{\Gamma\left(1/2-a-b\right)\Gamma\left(1+2b\right)} - x^{-2b} \frac{F\left(1/2-a-b, 1-2b;\ x\right)}{\Gamma\left(1/2+b-a\right)\Gamma\left(1-2b\right)} \right]. \quad (95)$$

Then, from (83), (88), (90) and (95) we derive

$$R(r) = C_1 \Gamma\left(1+2P\right)\Gamma\left(1/2-P-\lambda\right) \frac{\sin \pi(1+2P)}{\pi r} W_{\lambda,P}\big(\sqrt{-8mE}r\big). \quad (96)$$

As the Whittaker function $W_{a,b}(x)$ has an exponential damping [39]

$$W_{\substack{a,b \\ x\to\infty}}(x) \approx \mathrm{e}^{-1/2x} x^a, \quad (97)$$

Eq. (97) corresponds to a bound state wave function, which satisfies the fundamental condition (43) for $0 < P < 1/2$ interval.

Therefore, for $\tau = 0, \pm\infty$ the standard and additional levels are obtained from (94) with corresponding wave functions

$$R_{\mathrm{st}} = C_1 \rho^{-1/2+P}\, \mathrm{e}^{-\rho/2} F\left(1/2+P-\lambda, 1+2P; \rho\right), \quad (98)$$

$$R_{\mathrm{add}} = C_2 \rho^{-1/2-P}\, \mathrm{e}^{-\rho/2} F\left(1/2-P-\lambda, 1-2P; \rho\right). \quad (99)$$

For arbitrary $\tau \neq 0, \pm\infty$ the energy can be obtained from the transcendental equation (91), while the wave function is given by (96).

The unified form (96) is also a new result and is a consequence of the SAE procedure.

According to [39], our function (96) takes the following form:

$$R(r) = C_1 \Gamma\left(1+2P\right)\Gamma\left(1/2-P-\lambda\right) \times \\ \times \frac{\sin \pi\left(1+2P\right)}{\pi\rho}\, \mathrm{e}^{-\rho/2} \rho^{1/2-P} \Psi\left(\frac{1}{2}-\lambda-P,\ 1-2P;\ \rho\right), \quad (100)$$

where $\Psi(a,b,x)$ is one of the above-mentioned solutions, (86), namely, y_5. Its zeros are well-studied [39]: for real a, b (note, that in our case $a = 1/2-\lambda-P;\ b = 1-2P$ are real numbers) this function has finite numbers of positive roots. However, for the ground state there are three cases where this function has no zeros: 1) $a > 0$; 2) $a - b + 1 > 0$; 3) $-1 < a < 0$ and $0 < b < 1$. Only the last case is interesting for us, because $a = 1/2-\lambda-P;\ b = 1-2P$ and P is in the interval (47). It means

$$-1 < 1/2 - P - \frac{2m\alpha}{\sqrt{-8mE}} < 0. \quad (101)$$

In other words, the ground state energy, which is given by transcendental equation (91), must obey this inequality.

The wave function in the form of (100) is also new.

In monograph [38], energy levels for alkaline metal atoms are written in Ballmer's form

$$E_{n'} = -R\frac{1}{n'^2}, \tag{102}$$

where R is the Rydberg constant and n' is the effective principal quantum number

$$n' = n_r + l' + 1 \quad (n_r = 0, 1, 2\ldots), \tag{103}$$

while

$$l' = -1/2 \pm P = -1/2 \pm \sqrt{(l+1/2)^2 - 2mV_0}. \tag{104}$$

Only $(+)$ sign was considered in front of the square root until now. In [38], V_0 was considered to be small and after expansion of this root, approximate expression for the standard levels was derived

$$E_{\rm st} = -R\frac{1}{(n+\Delta_l)^2}, \quad n = n_r + l + 1, \tag{105}$$

where

$$\Delta_l \equiv \Delta_l^{\rm st} = -\frac{2mV_0}{2l+1} \tag{106}$$

is the so-called Rydberg correction (quantum defect) [23, 38].

As regards of additional levels, this procedure is invalid, because V_0 is bounded from below according to (44). Approximate expansion for additional levels is possible only for $l = 0$. We have in this case

$$P = \sqrt{\frac{1}{4} - 2mV_0} \approx \frac{1}{2}(1 - 4mV_0). \tag{107}$$

V_0 may be arbitrarily small, but different from zero, because in this case $P = 1/2$ and we have no additional levels.

One can easily obtain the existence condition of additional levels from (105) and (44) in diverse form

$$l < \Delta_l < l + 1. \tag{108}$$

If we use data of monograph [38], we obtain that for $l = 0$ states only Li, for $l = 1$ only K and for $l = 2$ only Cs satisfy (108) (i.e., they have additional solutions and it is necessary to carry out SAE procedure), and Na and Rb have no additional levels. The condition (108) helps us to determine which alkaline metals need SAE extension of Hamiltonian.

4.2. The Klein–Gordon Equation. Let us consider the Klein–Gordon equation in a central potential

$$\left(-\Delta + m^2\right)\psi(\mathbf{r}) = \left[E - V(r)\right]^2 \psi(\mathbf{r}). \tag{109}$$

After the separation of angles, we derive the radial form of this equation

$$\left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2} + m^2 - (E-V)^2\right] R(r) = 0, \tag{110}$$

and for the function $u = rR$, taking into account the condition (25), we have

$$u'' + \left[(E-V)^2 - m^2 - \frac{l(l+1)}{r^2}\right] u = 0. \tag{111}$$

It seems that even the Coulomb potential is singular by this equation. Now, the following classification must be accounted for this equation:

$$\lim_{r\to 0} rV(r) = 0 \text{ — regular}, \tag{112}$$

$$\lim_{r\to 0} rV(r) = -V_0 = \text{const} \text{ — singular}, \tag{113}$$

i.e., the area of application of Eq. (111) becomes narrower. It is applicable only for potentials, satisfying (112). Therefore, Eq. (111) may be used for potentials, which have less singularity than the Coulomb one, whereas in using of Eq. (110) no troubles appear.

4.3. "Hydrino" States in the Klein–Gordon Equation with the Coulomb Potential. We note that the problems of additional levels were discussed by other authors as well [39–42]. In particular, in [40] the Klein–Gordon equation is considered with $V = -\alpha/r$ Coulomb potential

$$R'' + \frac{2}{r}R' + \left[E^2 - m^2 - \frac{l(l+1)}{r^2} + \frac{2E\alpha}{r} + \frac{\alpha^2}{r^2}\right] R = 0. \tag{114}$$

The author underlines, that there must be levels below the standard levels (called "hydrino" eigenstates), but he/she did not perform the SAE procedure.

Let us consider this problem in more detail. First of all, note that Eq. (114) coincides with Eq. (82), but now

$$\rho = 2\sqrt{m^2 - E^2}, \quad \lambda = \frac{E\alpha}{\sqrt{m^2 - E^2}}, \quad P = \sqrt{(l+1/2)^2 - \alpha^2} > 0. \tag{115}$$

We must require $m^2 > E^2$ for bound states. Therefore, one can use all the previous relations from valence electron model taking into account the definitions (115). In particular, the SAE parameter now is

$$\tau = \frac{C_2}{C_1} \frac{1}{\left(2\sqrt{m^2 - E^2}\right)^P}, \tag{116}$$

and for eigenstates we have the following equation:

$$\frac{\Gamma(1/2 - \lambda - P)}{\Gamma(1/2 - \lambda + P)} = -\tau \left(2\sqrt{m^2 - E^2}\right)^P \frac{\Gamma(1-2P)}{\Gamma(1+2P)}. \tag{117}$$

This is a new form, that follows by SAE procedure in the Klein–Gordon equation. For the edge points we derive the standard and additional levels in analogy with (94):

$$E_{\text{st}} = \frac{m}{\sqrt{1 + \dfrac{\alpha^2}{(1/2 + n_r + P)^2}}}, \quad n_r = 0, 1, 2\ldots, \tag{118}$$

$$E_{\text{add}} = \frac{m}{\sqrt{1 + \dfrac{\alpha^2}{(1/2 + n_r - P)^2}}}, \quad n_r = 0, 1, 2\ldots \tag{119}$$

Exactly these (119) levels are called as "hydrino" levels in [39–42]. It is evident that the hydrino levels are analogical to $E_{\rm add}$ states of Eq. (94), but these two cases differ from each other. Particularly, it is possible to pass the limit $V_0 \to 0$ in Eq. (82) and obtain hydrogen problem. Usually, this limiting procedure is used in traditional textbooks to choose between two signs in (94), while in (114) coupling constants for both terms in potential terms are mutually proportional (α and α^2), and vanishing of one of them causes vanishing of another, so we turn to the free-particle problem instead of the Coulomb one. Moreover, as we mentioned above, in those papers [39–42] the SAE procedure was not used. They considered only two signs in front of square root in equation analogous to (94) and only (118) and (119) levels are considered, which correspond only to cases $\tau = 0$ and $\tau = \pm\infty$. Contrary to that case, we performed SAE procedure, derived Eq. (117) and take attention to the hydrino (when $\tau = \pm\infty$) problem.

The difference between standard and hydrino states manifests clearly in the nonrelativistic limit when $\alpha \to 0$, which must be performed with definite caution. The hydrino existence condition for such states folows from earlier constraints and the restriction $0 < P < 1/2$. It has the form

$$l(l+1) < \alpha^2, \tag{120}$$

and it is evident that for states with $l \neq 0$ in transition to the nonrelativistic $\alpha \to 0$ limit the additional (hydrino) states disappear. Therefore, we must consider only $l = 0$ states.

For the ground states ($n_r = l = 0$) we have

$$E^{(0)}_{\rm st} = \frac{m}{\sqrt{2}}\sqrt{1+\sqrt{1-4\alpha^2}}, \tag{121}$$

$$E_{\rm hyd} \equiv E^{(0)}_{\rm add} = \frac{m}{\sqrt{2}}\sqrt{1-\sqrt{1-4\alpha^2}}. \tag{122}$$

Expansion in powers of α gives

$$E^{(0)}_{\rm st} = m\left(1 - \frac{\alpha^2}{2} - \frac{\alpha^4}{8}\right), \tag{123}$$

$$E^{(0)}_{\rm hyd} = m\left(\alpha + \frac{\alpha^3}{2}\right). \tag{124}$$

It follows that the hydrino is a very tightly bound system and sensitive to the sign of α.

If we expand $l = 0$; $n_r \neq 0$ states till the order of α^2, we derive

$$E^{(0)}_{\rm st} = m\left(1 - \frac{\alpha^2}{2(n_r+1)^2}\right), \tag{125}$$

$$E^{(0)}_{\rm hyd} = m\left(1 - \frac{\alpha^2}{2(n_r)^2}\right). \tag{126}$$

Comparison of these two expressions shows that there appears some kind of degeneracy between the levels with $n_r + 1$ nodes of hydrino and energies for n_r nodes of standard states. This degeneracy disappears in the next order.

The fact that the additional (hydrino [39–42] or peculiar [43, 44]) states of the $(n_r + 1)$th $^1S_0$ state are nearly degenerate with the usual nth $^1S_0$ state may facilitate a tunneling transition. Our description by the unified function analogous of (96), as a result of SAE procedure, gives a possibility of interpolation between them.

4.4. The Yukawa Potential. As the last application of Eq. (21), let us consider the Yukawa potential. According to common viewpoint (see, e.g., [8], Ch. 28), the Yukawa potential is a spherically symmetric solution of the Helmholz wave equation

$$\nabla^2\varphi - \mu^2\varphi = 0. \tag{127}$$

If we do not pay attention to the appearance of the delta function, we would have a radial equation like [8]:

$$\frac{1}{r}\frac{d^2}{dr^2}(r\varphi) - \mu^2\varphi = 0, \tag{128}$$

the solution of which is $r\varphi = C\,\mathrm{e}^{\pm\mu r}$ and, in case of decaying asymptotic at infinity, the Yukawa potential follows

$$\varphi = C\frac{\mathrm{e}^{-\mu r}}{r}. \tag{129}$$

However, the application of the correct relation (21) gives

$$\nabla^2\frac{\mathrm{e}^{-\mu r}}{r} = \mu^2\frac{\mathrm{e}^{-\mu r}}{r} - 4\pi\delta^{(3)}(\mathbf{r})\,\mathrm{e}^{-\mu r}. \tag{130}$$

Interesting enough we found this equation in the earlier book [45]. It follows that the Yukawa potential is not a solution everywhere, but only outside the origin of coordinates. The Yukawa potential is the solution of the Helmholz wave equation with a source term on the RHS:

$$\nabla^2\varphi - \mu^2\varphi = -4\pi C\delta^{(3)}(r). \tag{131}$$

It was mentioned incorrectly in [7] that there is no need in imposing the boundary condition $u(0) = 0$ and it is sufficient to require regularity of solutions of the full radial equation. But it seems that, in this particular case, when the substitution (6) is applied, this requirement is equivalent to our restriction (25).

It is worthwhile to emphasize one important notion: of course, to make the substitution (6) is not necessary at all. One can use other substitutions in course of solution of Eq. (127). In this case, the conclusion of [7] becomes more transparent and leads to a new unexpected result.

Let us discuss this viewpoint in case of the Yukawa potential, i.e., of the Helmholz equation (127), rewriting it for the spherically symmetric solution as

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right]\varphi - \mu^2\varphi = 0, \tag{132}$$

and instead of (6) make the following substitution:

$$\varphi = \frac{\chi(r)}{\sqrt{r}}. \tag{133}$$

Denoting $z = \mu r$, we obtain the equation

$$\frac{d^2\chi}{dz^2} + \frac{1}{z}\frac{d\chi}{dz} - \left(1 + \frac{1}{4z^2}\right)\chi = 0. \tag{134}$$

The general solution of it is expressed in terms of modified Bessel functions [31]:

$$\chi(z) = aI_{1/2}(z) + bK_{1/2}(z), \quad z > 0. \tag{135}$$

Let us remember the asymptotic behavior for large and small arguments discussed above

$$\begin{aligned} I_P(z)_{z\to 0} &\approx \left(\frac{z}{2}\right)^P \frac{1}{\Gamma(P+1)}, \qquad I_P(z)_{z\to\infty} \approx \frac{\mathrm{e}^z}{\sqrt{2\pi z}}, \\ K_P(z)_{z\to 0} &\approx \left(\frac{z}{2}\right)^{-P} \frac{\Gamma(P)}{2}, \qquad K_P(z)_{z\to\infty} \approx \sqrt{\frac{\pi}{2z}}\,\mathrm{e}^{-z}. \end{aligned} \tag{136}$$

We conclude that the second solution must be chosen owing the falling behavior at large values of argument. Therefore, the solution of Eq. (132) is

$$\varphi = br^{-1/2}K_{1/2}(\mu r). \tag{137}$$

But [31],

$$K_{1/2}(z) = \sqrt{\frac{\pi}{2z}}\,\mathrm{e}^{-z} \tag{138}$$

or

$$\varphi(r) = c\frac{\mathrm{e}^{-\mu r}}{r}, \tag{139}$$

i.e., the Yukawa potential again.

However, as we saw above, unfortunately, this is not the solution *everywhere,* because of singularity at the denominator.

It seems that this fact has very far-reaching consequences. Namely, it turns out that the second function $K_P(z)$ is not a solution of the Bessel equation in spite of a widespread belief. Actually, a straightforward transition of one-dimensional results of mathematical physics (theory of special functions, where the Laplacian is present) does not give necessarily the same things in three or more dimensions.

CONCLUSIONS

We have found a singularity like the Dirac delta function in process of reduction of the Laplace equation in spherical polar coordinates, which was not mentioned earlier. The cornerstone in our consideration was a requirement of Dirac that the solution of the radial equation at the same time must be a solution of the full three-dimensional equation.

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. (25). Moreover, this condition is independent of whether the potential in the Schrödinger equation is regular or singular. The singular potential influences only the character of turning to zero of the radial function at the origin.

As regards of the full radial function $R(r)$, its equation is compatible with the primary (three-dimensional) equation (1) if the restriction (43) is satisfied. Therefore, to avoid the

misunderstandings, it is preferable to work with Eq. (4) in nonrelativistic and Eq. (110) in relativistic (Klein–Gordon equation) cases, correspondingly. Moreover, only nonsingular solutions of full radial equation must be taken into account, only they are compatible with the full three-dimensional equations.

The substitution (6) is convenient because the problem reduces to the one-dimensional one on the semi-axis. The real picture is as follows:

Particle, in principle, is able to move on the whole axis, but the effective potential is infinite for all negative values of argument. In this case, the wave function is identically zero on the whole negative axis. The condition $u(0) = 0$ guarantees continuity of the wave function at $r = 0$. This provides the compatibility with the full equation and the equivalence to one-dimensional problem [14].

The above-described situation takes place in spaces with dimensions three and more. Therefore, in all equations of mathematical physics, where the Laplacian is involved, after the separation of angular variables the singular solutions, generally speaking, would not be the solutions of the primary equations.

If we shut eyes to a term with the delta function and formally use the reduced radial equation, then all results derived till now with the aid of this equation for regular potentials with regular boundary condition at the origin, remain valid. It is not an insignificant result from practical point of view.

However, when one considers singular potentials, the use of equation for the full radial function $R(r)$ in parallel with the SAE procedure of the full radial Hamiltonian is necessary. The appropriate examples, considered above, elucidate this statement.

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