ISSN 1547-4771, Physics of Particles and Nuclei Letters, 2024, Vol. 21, No. 4, pp. 846–851. © Pleiades Publishing, Ltd., 2024.

PHYSICS OF ELEMENTARY PARTICLES AND ATOMIC NUCLEI. THEORY

The Boundary Condition for Reduced Radial Wave Function in Multi-Dimensional Schrodinger Equation

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Received October 13, 2023; revised January 28, 2024; accepted January 28, 2024

Abstract—We study the behavior of reduced radial wave function at the origin for multidimensional Schrodinger equation, where the angular variables are separated by using a hyperspherical formalism and the overall potential is chosen symmetric under rotations in full Euclidean space. It is shown that the rigorous restriction at the origin—Dirichlet boundary condition follows only in three-dimensional space, whereas in other dimensions (more than three) some physical reasonings are necessary in addition. According to our previous investigation the most appropriate is the Hermiticity of Hamiltonian or, equivalently, the conservation of particle number. In this case the preferable is a Dirichlet condition again for regular potentials, but for singular potentials (not soft) other conditions are also allowed together with it. In this meaning the three dimensions is a peculiar one.

Keywords: multidimensional Schrodinger equation, central potentials, Hyperspace coordinates, radial equation, boundary condition, regular and singular potentials

DOI: 10.1134/S1547477124701474

1. INTRODUCTION

During the last decades, number of papers have appeared about the Schrodinger equation in multi D-dimensional spaces [1–6]. For reduction of such a problem, usage of the hyperspherical formalism is the most expedient. It is noteworthy that besides the mathematical interest, this formalism has been successfully applied to various realistic physical problems, such as many particles problem, when N particles are placed in $D = 3N - 1$ dimensional Euclidian space [7, 8]. By its meaning D dimensions have some important peculiarities in comparison to 3-dimensions. Here the central symmetry means the using some collective potential, which has a symmetry concerning rotations relative to full D-dimensional space. Owing to that in the hyperspherical basis the separation of variables takes place and the one dimensional Schrodinger equation is derived with respect to a hyperradial variable leaving some traces of hyperspherical angles.

Multidimensional central potentials with a specific analytical form have been used [1–6] to interpret a number of physical phenomena and chemical processes, to explain the behavior of nanotechnological systems, etc.

The objective of the present article is to focus on special features of quantum mechanics in higher dimensions, specifically on the behavior of the radial wave function at the origin of coordinates. As well as we are dealing with a second order differential equation, to impose the suitable boundary conditions is necessary for determination the structure of spectra. Our aim in this article is not an application of this equation in some physical problems, which are considered already in sufficiently details (see, [1–8], and references there' in), but we want take attention only to one particular problem—the behavior of reduced wave function at the origin of coordinates. In all above mentioned papers, the boundary condition is postulated as a requirement for physical solution, but it is not specified which physical solution is taken into account. This problem will be considered below after remaining the main equations.

2. PRELIMINARIES

In arbitrary D-dimensions with hypercentral potential $V_D(r)$ the Schrodinger equation has the form [1] ($\hbar = m = 1$ units are chosen):

$$\left[-\frac{1}{2}\nabla_D^2 + V_D(r)\right]\psi_D(\mathbf{r}) = E_D\psi_D(\mathbf{r}), \qquad (1)$$

where $\mathbf{r}$ is a D-dimensional position vector, whose hyperspherical coordinates are $(r, \theta_1, \theta_2, \ldots\theta_{D-1})$ and r is a hyperradius, denoting the radial distance

$$r = \left(\sum_{i=1}^{D} x_i^2\right)^{1/2}. \qquad (2)$$

By $V_D(r)$ it is meant a "collective" (but not a pair) potential, which depends only on r. The Laplacian of this problem is expressed as

$$\nabla_D^2 = \frac{1}{r^{D-1}}\frac{\partial}{\partial r} r^{D-1}\frac{\partial}{\partial r} - \frac{\Lambda_{D-1}^2}{r^2}, \quad (3)$$

where Λ_{D-1} is a generalized squared angular momentum operator in D-dimensions. It obeys to the following equation

$$\Lambda_{D-1}^2 \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = l(l+D-2)\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}). \quad (4)$$

Here $\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})$ describes hyper spherical harmonics, which are characterized by quantum numbers $(l \equiv \mu_1, \mu_2, \mu_3, \ldots, \mu_{D-1} \equiv m) \equiv (l, \{\mu\})$. They are natural numbers $l = 0,1,2,\ldots$; $l \equiv \mu_1 \geq \mu_2 \geq \mu_3 \geq \ldots \geq \mu_{D-2} \geq |\mu_{D-1}| \equiv m$ and these objects obey to orthogonality conditions

$$\int\limits_{S_{D-1}} d\Omega_{D-1} \mathcal{Y}^*_{l',\{m'\}}(\Omega_{D-1})\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = \delta_{ll'}\delta_{\{\mu\},\{\mu'\}}. \quad (5)$$

Substituting

$$\psi_{E,l,\{\mu\}}(\mathbf{r}) = R_{El}(r)\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) \quad (6)$$

and accounting for (4), (5), it follows a hyperradial equation

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{D-1}{2r}\frac{d}{dr} + \frac{l(l+D-2)}{2r^2} + V_D(r)\right] \times R_{El}(r) = E_D R_{El}(r). \quad (7)$$

We see that by external view this equation does not differ from usual 3-dimensional radial equation, moreover it passes into it in case of $D = 3$. Therefore, we can study them in parallel to each other.

It is a usual practice to withdraw a first derivative term, which can be achieved by substitution

$$u_{El}(r) = r^{(D-1)/2} R_{El}(r). \quad (8)$$

After this, the equation reduces to the form

$$\left[-\frac{d^2}{dr^2} + V_{\text{eff}}(r)\right] u_{El}(r) = E_D(r) u_E(r), \quad (9)$$

where

$$V_{\text{eff}}(r) = V_D(r) + \frac{L(L+1)}{r^2} = V_D(r) + \frac{l(l+D-2)}{r^2} + \frac{(D-1)(D-3)}{4r^2} \quad (10)$$

and L is a "Grand orbital quantum number" or "hyperangular momentum"

$$L = l + \frac{D-3}{2}. \quad (11)$$

Therefore,

$$l(l+D-2) = L(L+1) - (D-1)(D-3)/4. \quad (12)$$

As it is mentioned in literature, *the physical solutions require* that $u_{El}(r) \to 0$, when $r \to 0$. Moreover, the normalization to unity of the total wave function leads to the following property of the reduced radial wave function $u_{El}(r)$:

$$\int\limits_0^\infty u_{El}^2(r)\, dr = 1. \quad (13)$$

Nevertheless, there is not specified which are the physical solutions, that guarantee such boundary behavior. Our aim is to establish under which physical conditions follows the above mentioned boundary behavior at the origin of coordinates. We see from Eqs. (9) and (10) that the Schroedinger equation describes the one-dimensional non-relativistic motion of a particle. It is worth noting that the D-dimensional Schrodinger equation is formally the same as the radial equation in three-dimensional case, but with the grand orbital momentum L. It has an essential difference because the grand orbital momentum L never vanishes in spaces of higher $D > 3$ dimensions, so the s-wave problem [9] does not arises here. The particle is subjected to the natural force coming from the potential $V_D(r)$ and two additional forces (10) with different physical origin: the centrifugal force associated with a nonvanishing hyperangular momentum, and a quantum fictitious force, associated to the quantum-centrifugal potential $(D-1)(D-3)/4r^2$ of purely dimensional origin. If we rewrite Eq. (10) in more transparent form as:

$$V_{\text{eff}}(r) = V_D(r) + \frac{(D+2l)^2 - 4(D+2l) + 3}{8r^2}, \quad (14)$$

it is seen that the effective potential depends on D and l through a special combination $(D+2l)$. Therefore, it appears that there is the interdimensional degeneracy phenomenon; this implies e.g., that for an arbitrary potential the energies of the 7-dimensional s-states are the same as those of the 5-dimensional p-states or the 3-dimensional d-states.

3. WAVE UNCTION'S BEHAVIOR AT THE ORIGIN OF COORDINATES

Let us mention that in 90th of the previous century the problem of self-adjointness of the reduced radial Hamiltonian in 3-dimensions was a subject of intensive considerations [10]. It is well known that the self-adjointness by itself is connected to the behavior of reduced wave function at the origin. Various possibilities (choice) of boundary conditions were considered, but the final agreement was not established, especially for singular potentials. Among them was the above

mentioned zero asymptotic (Dirichlet), but the problem of s-wave remained open. Some authors believed that the so-called Robin boundary condition [11] became preferable. We have previously proved [12] that the Dirichlet boundary condition appears to be unique for the reduced $u(r)$ function. The reason is the delta-like singularity, which appears in the Laplacian during the course of transition from total to reduced wave function. It is interesting to know if there is a such situation in multi dimensions.

As it was noted above, the multi-dimensional equation reduces to the 3-dimensional one after substitution $D = 3$, when $L \to l$ and we have for total radial function the equation:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} + V_3(r)\right] \times R_{El}(r) = E_3 R_{El}(r), \quad (15)$$

while the transformation (6) reads as: $u_{El}(r) = rR_{El}(r)$ or $R_E = u_E/r$.

After this substitution it follows that the radial part of Laplacian $\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right\}$ acts on the factor $1/r$:

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right\}\frac{u(r)}{r} = \frac{1}{r}\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right\}u(r) + u(r)\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right\}\left(\frac{1}{r}\right) + 2\frac{du}{dr}\frac{d}{dr}\left(\frac{1}{r}\right). \quad (16)$$

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

$$\frac{1}{r}\frac{d^2u}{dr^2} + u\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right) = \frac{1}{r}\frac{d^2u}{dr^2} - 4\pi\delta^{(3)}(\mathbf{r})u(r). \quad (17)$$

In consequence, the extra delta term arises in radial Laplacian and the equation for a reduced wave function takes the form

$$\left(-r\frac{d^2u(r)}{dr^2} + \frac{l(l+1)}{r^2}u(r)\right) + \delta(r)u(r) - 2[E - V_3(r)]ru(r) = 0. \quad (18)$$

The only way to avoid this extra term to derive the well-known equation for the reduced wave function is to impose a constraint $u(0) = 0$. Otherwise, we would force to include a delta like term in all potentials under consideration, which is physically meaningless. Only after using this constraint, which has a form of Dirichlet boundary condition, we return to the generally accepted reduced equation. Moreover, this fact is valid irrespective whether the potential is regular or singular and the problem of self-adjointness of reduced Hamiltonian is also solved automatically.

In regards to multidimensional case $D > 3$, analogous phenomenon does not occur, because in D-dimensions delta function appears in the following equation [13]

$$\Delta_r \frac{1}{r^{D-2}} = -(D-2)\Omega_D\delta^{(D)}(\boldsymbol{r}), \quad \Omega_D = \frac{2\pi^{D/3}}{\Gamma\left(\frac{D}{2}\right)}, \quad (19)$$

and the substitution (8) has nothing in common with this equation, except for $D = 3$. So, in multidimensional case there is no strong rigorous mathematical argument in favour of $u(0) = 0$.

Therefore, the following question arises: Is it possible, with the help of some regular steps to derive physically acceptable boundary condition for $D > 3$? To address this problem let us draw other physical suggestions, considered e.g., in [12], which can also be transferred to $D > 3$ spaces.

Usually, the consideration is rest on the normalization integral (13) and attempts to find maximal singular behavior at the origin, allowed by this condition and with the fundamental principles of quantum mechanics. In [12] we have considered some more common physical reasonings and saw that different physically acceptable arguments lead to diverse conclusions for the wave function behavior at the origin.

What happens in $D > 3$ dimensions?

From the continuity of $R(r)$ at the origin, according to (8) it follows $u(0) = 0$, insuring a finite probability at this point. Exactly this idea is used in any textbook on quantum mechanics. But it is desirable to weaken this requirement, because it is addressed to a single point and is so strong. One can require a finite differential probability in the spherical slice $(r, r + dr)$, or

$$|R|^2 r^{D-1}dr < \infty. \quad (20)$$

If $R \sim r^s$ at the origin, we must require $2s + D - 1 > 0$ and it follows that $s > (1 - D)/2$, or

$$u_{El}(r) = r^{(D-1)/2}R_{El}(r) = r^{\frac{D-1}{2}+s} = r^{\frac{1-D}{2}+s} \to u(0) = 0. \quad (21)$$

Another generalization is to require a finite total probability inside a sphere of small radius a,

$$\int_0^a |R|^2 r^{D-1}dr < \infty. \quad (22)$$

In this case more singular behavior is permissible, namely

$$\lim_{r\to 0} R(r) \approx \lim_{a\to 0} a^{-D/2+\varepsilon}, \quad (23)$$

where $\varepsilon > 0$ is a small positive constant and $\varepsilon \to 0$ at the end of the calculation. In this case

$$\lim_{r\to 0} u(r) \approx \lim_{a\to 0} a^{(D-1)/2}a^{-D/2+\varepsilon} \approx \lim_{a\to 0} a^{-1/2+\varepsilon} \to \infty. \quad (24)$$

The same constraint follows from the finite behavior of the norm

$$\int_0^\infty |R(r)|^2 r^{D-1} dr < \infty. \quad (25)$$

The strongest is the Pauli argument [14], namely, the time independence of the norm or conservation of the number of particles. To explore it, we follow the procedure described in [12]: In quantum mechanics the norm of the wave function is to be independent of time

$$\frac{d}{dt}\int \psi^* \psi dV = 0. \quad (26)$$

By using the time dependent Schroedinger equation, we transform this equation to

$$-\frac{i}{\hbar}\int \left[\psi^* (H\psi) - (H\psi^*)\psi\right] dV = 0. \quad (27)$$

Thus, the time independence of probability means that the Hamiltonian must be a Hermitian operator. By introducing the probability current density

$$\mathbf{J} = \mathrm{Re}\left[\psi^* \frac{\hbar}{im}\nabla\psi\right] \quad (28)$$

it is easy to show that

$$\mathrm{div}\mathbf{J} = \frac{i}{\hbar}\left[\psi^* (H\psi) - (H\psi^*)\psi\right]. \quad (29)$$

The equation for conservation of probability takes the form (after using the Gauss' theorem)

$$\frac{d}{dt}\int_V \psi^* \psi dV = -\int_V \mathrm{div}\mathbf{J} dV = -\int_S J_N dS, \quad (30)$$

where J_N is the normal component of the current relative to the surface.

If we assume that at the origin the Hamiltonian has a singular point, Gauss' theorem in the last equation is not applicable. We must exclude this point from the integration volume surrounded it by a small sphere of radius a. In this case, the surface integral is divided into a surface at infinity that encloses the total volume, and the surface of a sphere of radius a:

$$\lim_{a\to 0} a^{D-1}\int J_a d\Omega + \int_\infty J_N dS = 0, \quad (31)$$

where $d\Omega$ is an element of solid angle. In the D-dimensions we should have $dS = a^{D-1}d\Omega$. Because the wave function must vanish at infinity, the second term goes to zero. If we substitute

$$J_a = \frac{i\hbar}{2m}\left(\left[\psi\left(\frac{\partial\psi^*}{\partial r}\right) - \psi^*\left(\frac{\partial\psi}{\partial r}\right)\right]\right)_{r=a} \quad (32)$$

and assume $\psi = \tilde{u}/r^s$, where $\tilde{u}$ is regular at $r \to 0$, we obtain

$$\lim_{a\to 0}\frac{a^{D-1}}{a^{2s}}\int\left(\tilde{u}\frac{\partial\tilde{u}^*}{\partial r} - \tilde{u}^*\frac{\partial\tilde{u}}{\partial r}\right)_{r=a} d\Omega = 0. \quad (33)$$

This equation is satisfied if $s < (D-1)/2$. It follows that $R(r)$ does not diverge more rapidly than $1/r^s$, but now $s < (D-1)/2$, which means that

$$\lim_{r\to 0} u(r) \approx \lim_{r\to 0} r^{-s+\frac{D-1}{2}} \to 0. \quad (34)$$

Consequently, we see that different physically acceptable arguments lead to diverse conclusions for the wave function behavior at the origin. Namely, a finite norm allows for a certain divergent behavior of $u(r)$, but the time independence of the norm gives vanishing behavior. We are inclined to think that this last requirement is most fundamental because it is related to hermiticity of the Hamiltonian and the vanishing of the reduced wave function is accepted as valid. Moreover, it is in accord to the three dimensional case. In this context, one can remember the opinion of W. Pauli [14], that "An eigenfunction for which $\lim_{r\to 0}(rR) \neq 0$, is not admissible, though for such function $\int_0^\infty |R|^2 r^2 dr$ exists".

4. SINGULAR POTENTIAL AND THE SELF-ADJOINT EXTENSION (SAE)

The behavior of reduced wave function, when r turns to the origin of coordinates evidently depends on potential $V_D(r)$ under consideration. The authors of [1–6] believe that "the physical solutions require that $u_{El}(r) \to 0$ when $r \to 0$ and ∞". But this opinion may not be correct in general without considering singular properties of the outcome potential $V_D(r)$. It must be clarified which physical solutions are meant by authors.

From this point of view the following classification is known for the Schroedinger equation [9] (It is natural, that this classification is the same in any dimensions):

• (1) **Regular potentials.** They behave as

$$\lim_{r\to 0} r^2 V_D(r) = 0. \quad (35)$$

For which solution of the equation

$$\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + V_D(r)\right)u_D(r) = E_D u_D(r) \quad (36)$$

at the origin behaves like

$$u(r) \underset{r\to 0}{=} C_1 r^{L+1} + C_2 r^{-L}. \quad (37)$$

Because L always is positive when $D \geq 4$, the second solution must be discarded, i.e., $C_2 = 0$.

Therefore, all singularities may be contained into $V_D(r)$.

• (2) **Strong singular potentials,** for which

$$\lim_{r\to 0} r^2 V_D(r) = \pm\infty. \quad (38)$$

For them, the "falling to the center" happens and is not interesting for us now.

• (3) **"Soft-singular" potentials,** for which

$$\lim_{r\to 0} r^2 V_D(r) = \pm V_0, \quad (V_0 = \text{const} > 0). \quad (39)$$

Here the $(+)$ sign corresponds to repulsion, while the $(-)$ sign—to attraction. For such potentials, the wave function has the following behavior

$$\lim_{r\to 0} u(r) = A_1 r^{1/2+P} + A_2 r^{1/2-P} = u_{\text{st}} + u_{\text{add}}, \quad (40)$$

where

$$P = \sqrt{(L+1/2)^2 - 2V_0}. \quad (41)$$

In the region $0 < P < 1/2$ the second solution (23) also satisfies Dirichlet boundary condition and hence it must be retained in general and therefore the self-adjoint extension need to be performed [15]. As for the region $P \geq 1/2$, only the first (standard or regular) solution remains. Recalling the relation (9). One can rewrite P as follows

$$P = \sqrt{\left[l + \frac{D-2}{2}\right]^2 - 2V_0}, \quad (42)$$

or existence of the second (additional) solution can take place when

$$\left[l + \frac{D-2}{2}\right]^2 - 1/4 < 2V_0 \quad (43)$$

i.e. with growth of dimension the restriction on V_0 increases. Therefore, the appearance of extra (so-called, hydrino) states becomes more limited [15].

5. CONCLUSIONS

In this article, we consider the problem of boundary condition of the radial wave function in an arbitrary dimensional quantum mechanics for generalized central potentials. We have shown that in many $(D > 3)$-dimensions there are no rigorous reasonings to fix boundary condition at the origin of coordinates, contrary to 3-dimensions. But from the time independence of the norm (which means a conservation of particle number in nonrelativistic quantum mechanics, and at the same time, guarantee self-adjointness of the Hamiltonian) the vanishing (i.e., Dirichlet) boundary condition is strongly motivated for both regular as well as singular potentials. For singular potentials (not soft) there remain possibility employing other conditions as well. In this respect, remarkably enough, 3-dimensions stand out sharply against the other dimensions in the sense that only in $D = 3$-dimensions the reducing procedure automatically gives the boundary condition, $u(0) = 0$ and moreover, corresponding Hamiltonian becomes a self-adjoint operator (For details, see [15]).

FUNDING

This work was supported by ongoing institutional funding. No additional grants to carry out or direct this particular research were obtained.

CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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