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Physics

Reduced Radial Wavefunction Asymptotic Behavior at the Origin of Multidimensional Spherically Symmetric Schrodinger Equation

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We study the behavior of reduced radial wave function at the origin for multidimensional Schrodinger equation, when angular variables are separated by using hyperspherical formalism and the overall potential is chosen symmetric under rotations in full Euclidean space. It is shown that rigorous restriction at the origin - Dirichlet boundary condition arises only from three-dimensional space, whereas in other dimensions (more than three) some physical conditions are necessary. The most appropriate is the hermiticity of Hamiltonian or, equivalently, the conservation of particles number. In this case the Dirichlet condition is again preferable for regular potentials, but for singular potentials (not soft) other conditions (e.g. Robin) are also allowed together with it. In this regard the three-dimension space is a peculiar one. *© 2023 Bull. Georg. Natl. Acad. Sci.*

multidimensional Schrodinger equation, hyperspace coordinates, boundary condition

During the last decades, a number of papers 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. Besides the mathematical interest, this formalism has been applied to many particles problem, when N particles are placed in $D = 3N - 1$ dimensional Euclidian space [7,8]. By its meaning D-dimension has some important peculiarities in comparison with 3-dimensions. Here the central symmetry is meant using some collective potential, which has a symmetry concerning rotations relative to full D-dimensional space. In the hyperspherical basis the one dimensional Schrodinger equation is derived with respect to a hyperradial variable leaving some traces of hyperspherical angles. Multidimensional central potentials were used to interpret a number of physical phenomena and chemical processes, to explain the behavior of nanotechnological systems, etc.

The objective of the present work 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 we are dealing with the second order differential equation to impose the suitable boundary conditions are necessary for structure determination of spectra. Our aim is not an application of this equation in the physical problems, which are considered in details [1-8], but we want to take attention only to one particular problem; the behavior of reduced wave function at the origin. In the 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.

Preliminaries

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

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

where $V_D(r)$ is a hyperspherical potential, invariant under full D space-rotations.

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

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

After this, the equation reduces to the form:

$$\left[-\frac{d^2}{dr^2} + V_{eff}(r)\right] u_{El}(r) = E_D(r) u(r), \tag{3}$$

where

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

and L is a "grand orbital quantum number"

$$L = l + \frac{D-3}{2}, \tag{5}$$

therefore

$$l(l+D-2) = L(L+1) - (D-1)(D-3)/4. \tag{6}$$

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

$$\int_0^\infty u_{El}^2(r)\,dr = 1. \tag{7}$$

Nevertheless, there is not specified which are the physical solutions, that guarantee such boundary behavior. Our aim is to establish under which physical conditions the above mentioned boundary behavior follows. We see from Eqs. (3) and (4) that the Schrodinger equation describes the one-dimensional non-relativistic motion of the particle. The D-dimensional Schrodinger equation is formally the same as the radial equation in three-dimensional case, but with the grand orbital momentum L. The particle is subjected to the natural force coming from the potential $V_D(r)$ and two additional forces (4) with different physical origin: the centrifugal force associated with nonvanishing hyperangular momentum and quantum fictitious force, associated to the quantum-centrifugal potential $(D-1)(D-3)/4r^2$ of purely dimensional origin. If we rewrite Eq. (4) in more transparent form as:

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

we see that $V_{eff}(r)$ depends on D and l through special combination $(D+2l)$. Therefore, it appears that there is an interdimensional-degeneracy phenomenon. This implies that e.g., 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.

Wave Function Behavior at the Origin of Coordinates

Let us mention that in the 1990s, the problem of self-adjointness of the reduced radial Hamiltonian was a subject of intensive considerations [9]. It is well known that the self-adjointness by itself is connected to the behavior of reduced wave function at the origin. Various possibilities of boundary conditions were considered, but the final agreement was not established, especially for singular potentials. Among them was the above zero asymptotic condition (Dirichlet), but the problem of s-wave remained open (Robin boundary condition became preferable). We proved [10] that the Dirichlet boundary condition appears to be unique. The reason is the delta-like singularity, which appears in Laplacian in the course of transition from total to reduced wave function. Is there such mechanism in multi dimensions?

Note that the multi-dimensional equations reduce to the 3-dimensional ones after substitution $D=3$. In this case, $L \to l$ and we have for total radial function the equation:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} + V_3(r) \right] R_{El}(r) = E_3 R_{El}(r), \tag{9}$$

while the transformation (2) reads as: $u_{El}(r) = rR_{El}(r)$ or $R = u/r$.

After this substitution the radial part of Laplacian acts on the factor $1/r$, which is a three dimensional delta function. So, the term $\delta(r)u(r)$ appears in the reduced equation, which at this step looks like [10]

$$\left(-r\frac{d^2u(r)}{dr^2} + \frac{l(l+1)}{r^2}u(r) \right) + \delta(r)u(r) - 2\left[E - V_3(r)\right]ru(r) = 0. \tag{10}$$

The only way to avoid this extra term is a constraint $u(0)=0$. 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.

In regards to multidimensional case D>3, analogous phenomenon does not occur, because in D-dimensions delta function appears in the following equation [11]

$$\Delta_r \frac{1}{r^{D-2}} = -(D-2)\Omega_D \delta(\boldsymbol{r}), \qquad \Omega_D = \frac{2\pi^{D/3}}{\Gamma\left(\frac{D}{2}\right)} \tag{11}$$

and the substitution (2) has nothing in common with this equation, except for $D=3$.

Therefore, the following question arises: Is it possible, with the help of some regular steps to derive physically acceptable boundary condition? To address this problem let us draw other physical suggestions, considered e.g., in [10], which can also be transferred to $D>3$ spaces.

Usually, the normalization condition is considered (7) and tried to find maximal singular behavior, consistent with this condition and with the fundamental principles of quantum mechanics. In [10] we considered some more common physical conditions:

We saw that different physically acceptable arguments lead to derive 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 the most fundamental because it is related to hermiticity of the Hamiltonian and the vanishing of the reduced wave function is accepted as valid.

In this context, one can remember the opinion of W. Pauli [12: 45], 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''

Singular Potential and Self-Adjoint Extension (SAE)

The behavior of the 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. It must be clarified, which physical solutions are meant.The following classification is known [13] (It is natural, that this classification is the same in any dimensions):

Regular potentials. They behave as

$$\lim_{r\to 0} r^2 V_D(r)=0. \tag{12}$$

For which solution of the equation

$$\left(-\frac{d^2}{dr^2}+\frac{L(L+1)}{r^2}+V_D(r)\right)u_D(r)=E_D u_D(r) \tag{13}$$

at the origin behaves like

$$\underset{r\to 0}{u(r)}=C_1 r^{L+1}+C_2 r^{-L}. \tag{14}$$

Because L 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) **Singular potentials,** for which

$$\lim_{r\to 0} r^2 V_D(r)=\pm\infty. \tag{15}$$

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

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

$$\lim_{r\to 0} r^2\, V_D(r)=\pm V_0, \quad (V_0=const>0). \tag{16}$$

Here the (+) sign corresponds to repulsion, while the (–) sign – to attraction. For such potentials, the wave function behaves as $\lim_{r\to 0} u(r)=A_1 r^{1/2+P}+A_2 r^{1/2-P}=u_{st}+u_{add}$, where

$$P=\sqrt{(L+1/2)^2-2V_0}. \tag{17}$$

For $0 < P < 1/2$ the solution $u_{add} = A_2 r^{1/2-P}$ satisfies Dirichlet boundary condition and it must be retained in general and therefore, the self-adjoint extension need to be performed [14]. For $P \geq 1/2$, only the first (standard or regular) solution remains. Recalling the relation (5), one can rewrite P as follows

$$P = \sqrt{\left[l + \frac{D-2}{2}\right]^2 - 2V_0}, \tag{18}$$

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

$$\left[l + \frac{D-2}{2}\right]^2 - 1/4 < 2V_0, \tag{19}$$

i.e. with the growth of dimension the restriction on V_0 increases. Therefore, the appearance of extra (so-called, hydrino) states becomes more limited [14].

Conclusions

In this paper, we consider the problem of boundary condition of the radial wave function in an arbitrary dimensional quantum mechanics for 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 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 remains possibility employing other conditions. In this respect, remarkably enough, 3-dimensions stand out sharply against the other dimensions in the sense that only in 3-dimensions the reducing procedure automatically gives the condition $u(0) = 0$ and corresponding Hamiltonian is self-adjoint operator (for details, see [14]).

ფიზიკა

დაყვანილი რადიალური ტალღური ფუნქციის სათავეში ასიმპტოტური ყოფაქცევა შრედინგერის მრავალგანზომილებიანი სფერული სიმეტრიის განტოლების შემთხვევაში

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*** ივანე ჯავახიშვილის სახ. თბილისის სახელმწიფო უნივერსიტეტი, ზუსტ და საბუნიბისმეტყველო მეცნიერებათა ფაკულტეტი, ფიზიკის დეპარტამენტი; მაღალი ენერგიების ფიზიკის ინსტიტუტი, თბილისი, საქართველო*

ჩვენ ვსწავლობთ მრავალგანზომილებიანი შრედინგერის განტოლების დაყვანილი ტალღური ფუნქციის ყოფაქცევას სათავეში, როცა კუთხური ცვლადები განცალკევებულია ჰიპერსფერული ფორმალიზმის გამოყენებით და საერთო პოტენციალი არის ევკლიდეს სივრცეში სრული ბრუნვების მიმართ სიმეტრიული. ნაჩვენებია, რომ მკაცრი მათემატიკური შეზღუდვა ყოფაქცევაზე სათავეში – დირიხლეს სასაზღვრო პირობა გამომდინარეობს მხოლოდ 3-განზომილებიან სივრცეში, მაშინ, როცა სხვა განზომილებებში (სამზე მეტი) აუცილებელია დამატებით გარკვეული ფიზიკური პირობები, ყველაზე მისადაგებული არის ჰამილტონიანის ერმიტულობა, ანუ ნაწილაკთა რიცხვის შენახვა. მოცემულ შემთხვევაში უპირატესია კვლავ დირიხლეს პირობა რეგულარული პოტენციალებისთვის, ხოლო სინგულარული პოტენციალებისთვის (არა რბილი) მასთან ერთად დასაშვებია სხვა სასაზღვრო პირობებიც (მაგ., რობინის). ამ თვალსაზრისით სამგანზომილებიანი სივრცე განსაკუთრებულია.

REFERENCES

1. Dehesa J.S. (2021) Spherical-symmetry and spin effects on the uncertainty measures of multidimensional Quantum Systems with central potentials. *Entropy*., **33**:607.
2. Al-Jaber S. (2016) Uncertainty relations for some central potentials in N-dimensional space. *Applied Mathematics*, **7**:508.
3. Paz G. (2001) On the connection between the radial momentum operator and the Hamiltonian in *n* dimensions. *Eur.J.Phys*., **22**:337.
4. Sanchez-Moreno P., Gonzalez-Ferez R., Dehesa J.S. (2006) Improvement of the Heisenberg and Fisher-information-based uncertainty relations for *D*-dimensional central potentials. *New Journ. of Physics*., **8**: 330.
5. Dong S., Sun G. (2004) The Schrödinger equation with a Coulomb plus inverse-square potential in D-Dimensions. *Physica Scripta*., **70**:94.
6. Nieto M. (1979) Hydrogen atom and relativistic pi-mesic atom in *N*-space dimensions. *Am. J. Phys.,* **47**:1067.
7. Ballot J., Ripelle F.(1986) Application of the hyperspherical formalism to the trinucleon bound state problems. *Annals of Physics*., **127**:62.
8. Khelashvili A., Khmaladze V., Chachava D. (1985) Many-particle problem with logarithmic potentials and its application to quark bound states. *Sov. J. Teoreticheskaya i Matematicheskaya Fizika.*, **62**: 136. M. (in Russian).
9. Gitman D., Tyutin I., Voronov B. (2012) Self-adjoint extensions in quantum mechanics (Springer, New York).
10. Khelashvili A. and Nadareishvili T. (2011) What is the boundary condition for the radial function of the Schrodinger equation. *Am.J. Physics.*,**79**:668.
11. Gel'fand I., Shilov G. (1962) Generalized functions. Acad. Press, New York.
12. Pauli W. (1980) General principles of quantum mechanics Springer-Verlag. Translated in New York.
13. R. Newton R. (2002) Scattering theory of waves and particles*,* 2nd ed. Dover Publ., New York.
14. Khelashvili A. and Nadareishvili T. (2015) 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. *Physics of Particles and Nuclei Letters.,* **12**:11.

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