

ONE OF THE WAYS OF THE SOLUTION OF SCHRÖDINGER EQUATION FOR THREE PARTICLES SYSTEMS WITH INVERSE SQUARE PAIR POTENTIAL

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ABSTRACT. In accordance with the solution of Schrödinger equation for three-particle system with inverse square distance dependent pair potential the bound state is not realized at all i.e. the ground state energy equals to $-\infty$, which is physically meaningless. The reason of this fact is that the potential is critically singular.

The article studies how to solve Schrödinger equation for three particle system of inverse square distance dependent pair potential by modified hyperspherical function method (MHFM) that gives Hamiltonian corresponding to Schrödinger equation and at the same time includes the similar to the Coulomb potential and critically singular potential. The solution of the Schrödinger equation, which includes this kind potential with corresponding boundary conditions is given in any quantum mechanical book. This solution has been given exact physical results and shown that, in the first approximation binding energy of the system changes monotonically by global quantum number.

However, as we remarked above, in this case similar to the Coulomb potential appeared in Schrödinger equation. So the result does not correspond to the initially studied system (only to the inverse square distance dependent pair potential for three particle system).

1 INTRODUCTION

A number of physical phenomena can be described by singular potentials [1-9], and especially interesting among them is the inverse square distance dependent pair potential (critical singular potential),

because it can be used as independently as with the other power singular potentials [10-14] in different areas of physics.

Schrödinger equation for two particle system with such potential has been studied in ref. [15,16].

Solution of Schrödinger equation with critically singular potential can be achieved by renumbering method, which initially had been formed by Wilson [17], when he carried out calculation by the quantum field theory and the renumbering the inverse square potential has become the parameter cutoff. This parameter cutoff used to inverse square potential has got not only physical result [16,18] but also possibility to explain the break of quantum anomaly and its experimental results [19] (where was observed interaction between dipole and electron.). In spite of that the inverse square potential system was limited: 1) by two particle systems in ND space, when $N \geq 1$; 2) by three and multi-particle systems in 1D space.

So the investigation of three particle-system as independent critical singular potential and with its other power singular potentials in 2D and 3D spaces will extend knowledge and it will be more precise definition about this potential and also will extend the sphere of use of this potential.

2 FORMULATION OF THE PROBLEM

We considered the potential of inverse square distance dependence (critical singular potential):

$$V(r) = a \cdot r^{-2}. \quad (1)$$

The radial parts of Schrödinger equation with two-particle system (1) is as following:

$$R'' + \frac{2}{r} R' + \frac{\lambda}{r^2} R + k^2 R = 0, \quad (2)$$

where R is a radial part of a wave function:

$$\lambda = \frac{2\mu\beta}{\hbar^2} - \ell(\ell+1)$$

and if $V(r) \sim 1/r^2$ was in whole space, then bound state was not realized in case of $\lambda < 1/4$ at all. And when $\lambda > 1/4$, a particle “falls into the center” (ground state energy equals to $-\infty$) and so it is physically meaningless [15,16].

In ref. [20,21] three particle system has been studied with pair of interaction of the same expression (1) between particles. Hyperspherical function method has been used [22]. However, after using this method we obtained system of the coupled differential equations. Let us consider one equation from this system for the hyperradial wave function in 2D [20] and it is expressed as follows:

$$\left(\frac{\partial^2}{\partial \rho^2} + \frac{3}{\rho} \frac{\partial}{\partial \rho} - \left[\chi^2 + \frac{K(K+2)}{\rho^2} \right] \right) \chi_K(\rho) = \frac{2\mu}{\hbar^2 \rho^2} J_K \chi_K(\rho), \quad (3)$$

where K – is the particles hypermoment.

$$\chi^2 = -\frac{2\mu}{\hbar^2} E$$

if define λ as follows:

$$\lambda = -K(K+2) - \frac{2\mu}{\hbar^2} J_K$$

(3) and (2) are analogous. If $V(r) \sim 1/r^2$ is in the whole space then bound state is not realized in case of $\lambda < 1$ at all. And when $\lambda > 1$ then a particle “falls into the center” (ground state energy equals $-\infty$) and so it is physically meaningless.

From [21] paper it is clear that after using this method only in the first approximation from infinitely continued equation system for the hyperradial wave function in 3D is as follows:

$$\left(\frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial}{\partial \rho} - \left[\chi^2 + \frac{K(K+4)}{\rho^2} \right] \right) \chi_K(\rho) = \frac{2\mu}{\hbar^2 \rho^2} J_K \chi_K(\rho), \quad (4)$$

if we define λ as follows:

$$\lambda = -K(K+4) - \frac{2\mu}{\hbar^2} J_K,$$

(4) and (2) are analogous. But if $V(r) \sim 1/r^2$ was in the whole space then bound state was not realized in case of $\lambda < 4$ at all. And when $\lambda > 4$ then a particle “falls into the center” (ground state energy equal to $-\infty$) and so it is physically meaningless.

So despite existence of solutions of (3) and (4) equations characterized the solution of Schrödinger equation corresponding to two-particle systems we have got for them an unbound system or physically meaningless results.

So the problem solution by Schrödinger equation for three-particle system which contains (1) potential where the non-model approach can be used must be very interesting.

It has been investigated three particle system with the same potential using of modified hyperspherical function method [4-6] (see chapter 3) that gives Schrödinger equation with corresponding Hamiltonian including the same Coulomb potential. So as a result of using MHFM on three-particle system in 2D space with first approximation the following equation was obtained:

$$\left(\frac{\partial^2}{\partial \rho^2} + \left(\frac{3}{\rho} - W'_2 \right) \frac{\partial}{\partial \rho} + \frac{3W'_2 + W'_3}{\rho} + \left(\chi^2 + W'_6 \right) - \frac{2\mu}{\hbar^2} \frac{K(K+2) + J_0}{\rho^2} \right) \psi(\rho) = 0 \quad (5)$$

(all quantity is given in chapter 3).

From (5) it is clearly seen that it includes the same Coulomb potential (the third component in the bracket).

Analogically MHFM on three particle system in 3D space was used and as a result we have got:

$$\left[\frac{\partial^2}{\partial \rho^2} + \left(\frac{5}{\rho} - W'_2 \right) \frac{\partial}{\partial \rho} + \frac{3W'_2 + W'_3}{\rho} + \right. \\ \left. + \left(\kappa^2 + W'_6 \right) - \frac{2\mu}{\hbar^2} \frac{K(K+1) + J_0}{\rho^2} \right] \psi(\rho) = 0 \quad (6)$$

(all quantities in equation have been explained in chapter 3).

Also from (6), it is clearly seen that it includes the same Coulomb potential (the third component in the bracket).

Corresponding to boundary conditions solution of Schrödinger equation with Coulomb potential is given in any quantum mechanical book. Solutions of (5) and (6) equations are given in [20,21].

The solution had taken into account asymptote behavior of solution. In particular, when $\rho \rightarrow 0$ the solution has been found with $\Psi \sim \rho^\sigma$:

$$\sigma = -2 + \left[(K+2)^2 - \frac{2\mu}{\hbar^2} J_0 \right]^{1/2} \quad \text{in 3D space;} \quad (7)$$

$$\sigma = -1 + \left[(K+1)^2 - \frac{2\mu}{\hbar^2} J_0 \right]^{1/2} \quad \text{in 2D space.} \quad (8)$$

Here and later on (for (18) and (19) the same expressions are being obtained) it should be taken into account that interaction constants in three particle system is negative when $a_{ij} < 0$, (calculation of J_0 in 2D and 3D spaces given in [20,21]). As seen from appendix, J_0 was negative for any negative value of a_{ij} . Though in (7) and (8) equations the expression under root will be positive for any negative values of a_{ij} . The expressions of bound state energy of system was as following: in 2D space

$$E_N = -\frac{\hbar^2}{8\mu} \left[\left(\frac{12W'_2 + 4W'_3 - W'_2(3 + 2\sigma - 2N)}{3 + 2\sigma - 2N} \right)^2 - W_2^2 + 4W'_6 \right], \quad (9)$$

and in 3D space

$$E_N = -\frac{\hbar^2}{8\mu} \left[\left(\frac{12W'_4 + 4W'_3 - W'_2(2\sigma + 5 - 3N)}{2\sigma + 5 - N} \right)^2 - W_2^2 + 4W'_6 \right]. \quad (10)$$

The solution obtained from (9) and (10) by Schrödinger equation, in first approximation, has shown that binding energy of the system changes monotonically according to global quantum number.

Although bound state energies of three-particle system obtained using MHFM are finite and not meaningless, the question is how real they are.

3 PROBLEM SOLUTION

The main idea of the modified hyperspherical function method (MHFM) [4-6] is that the wave function is Ψ presented as the product of two functions, where the first is the main hyperspherical function and the second is the “correlation function” - $\zeta = \exp(f)$ that defined by singularity and clustering properties of the wave function and it is equal to:

$$f = -\sum_{i=1}^3 \gamma_i r_i, \quad (11)$$

where r_i is a distance between the particles and γ_i is determined according to physical considerations. Considering relation between the three different sets of the given in [22] Jacob's coordinates, (11) could be rewritten as following:

$$\sum_{i=1}^3 \gamma_i z_i = \rho(G_1 \cos \alpha + G_2 \sin \alpha), \quad (12)$$

where

$$G_1 = \gamma_1 + \gamma_2 \cos(\phi_{23} + \phi_{31}) - \gamma_3 \cos \phi_{31};$$

$$G_2 = \gamma_2 \sin(\phi_{23} + \phi_{31}) - \gamma_3 \sin \phi_{31}. \quad (13)$$

ϕ_{23} , ϕ_{31} – angles were defined by [22]. Taking into account the above and simple transformations we obtained Schrödinger equation in 2D space (5), where

$$W'_2 = (G_1 - G_2) \cdot \frac{21\sqrt{6}}{8}; \quad W'_6 = G_1^2 + G_2^2;$$

$$W'_3 = W'_2 + 21\sqrt{6}(0,25G_1 + G_2) \quad (14)$$

and in 3D space (6), where

$$W'_2 = (G_1 - G_2) \cdot \frac{4}{15}; \quad W'_6 = G_1^2 + G_2^2;$$

$$W'_3 = G_1 \left(\frac{4}{15} - \frac{3\pi}{8} \right) - \frac{42}{105} G_2. \quad (15)$$

As we already have denoted, application of hyperspherical function modified method for three particle-system carried out with (1) type pair interaction (as it is given in previous chapter for 2D and 3D spaces) gives Schrödinger equations that are similar with effective Hamilton potentials including the potential similar to Coulomb's potential.

[23] was regards in 3D space with pair interaction:

$$\left(\frac{a}{r^2} + \frac{b}{r} \right). \quad (16)$$

This equation can be exactly solved by Schrödinger equation without MHFM.

Without MHFM, bound energy in 2D and 3D space is obtained analytically:

$$E = -\frac{\hbar^2}{2m} \left(\frac{V_c}{2N + 2\lambda} \right)^2, \quad (17)$$

where

$$\lambda = \frac{1}{2} + \sqrt{(K+1)^2 + W_1}; \quad (\text{in 2D space});$$

$$\lambda = \frac{1}{2} + \sqrt{(K+2)^2 + W_1}, \quad (\text{in 3D space});$$

$N = (\lambda + W/(2\chi))$; V_c and W_1 are the values of the calculating results the similar of the Coulomb potential and the square inverse potential related with an angular (arc) integral.

Using MHFM for (16) potential the Schrödinger equation of three particles system with pair interaction between particles has been obtained in 2D space

$$\left(\frac{\partial^2}{\partial \rho^2} + \left(\frac{3}{\rho} - W'_2 \right) \frac{\partial}{\partial \rho} + \frac{3W'_2 + W'_3 - V_c}{\rho} + \right. \\ \left. + \left(\chi^2 + W'_6 \right) - \frac{2\mu}{\hbar^2} \frac{K(K+2) + J_0}{\rho^2} \right) \Psi(\rho) \quad (18)$$

and in 3D space [23]

$$\left(\frac{\partial^2}{\partial \rho^2} + \left(\frac{5}{\rho} - W'_2 \right) \frac{\partial}{\partial \rho} + \frac{3W'_2 + W'_3 - V_c}{\rho} + \right. \\ \left. + \left(\chi^2 + W'_6 \right) - \frac{2\mu}{\hbar^2} \frac{K(K+1) + J_0}{\rho^2} \right) \Psi(\rho) = 0, \quad (19)$$

where the marks explained in (14) and (15) and $V_c = \frac{2\mu}{\hbar^2} J_1$; Behavior of (18) and (19) were still defined by (7) and (8), where the expression under root was did not depend on b , because b depends only on J_1 . J_1 – is the value of the calculation result of an angular (arc) integral related to the second component of expression (16):

$$J_{KK'LL'MM'}^{l_1 l_2 l_1' l_2'} = \int \Phi_{KLM}^{*l_1 l_2}(\Omega_i)(b_{12}r_{12}^{-1} + b_{13}r_{13}^{-1} + b_{23}r_{23}^{-1})\Phi_{K'L'M'}^{l_1' l_2'}(\Omega_i)d\Omega$$

in the first approximation.

In solution of (18) and (19) account has been taken of an asymptote behavior of the solution, in particular when $\rho \rightarrow 0$. Then solution has been found with $\Psi \sim \rho^\sigma$ where σ in 2D and 3D spaces expressed by (7) and (8) relationships. From (7) and (8) it is clearly seen that the expression under root does not depend on constant (b_{ij}).

Solution of (18) and (19) equations gives same of the bound expressions in 2D space:

$$E_N = -\frac{\hbar^2}{8\mu} \left[\left(\frac{12W_2' + 4W_3' - 4V_C - W_2'(3 + 2\sigma - 2N)}{3 + 2\sigma - 2N} \right) - W_2^2 + 4W_6' \right] \quad (20)$$

in 3D space:

$$E_N = -\frac{\hbar^2}{8\mu} \left[\left(\frac{4(3W_2' + W_3' - V_C) - W_2'(2\sigma + 5 - 3N)}{2\sigma + 5 - N} \right)^2 - W_2^2 + 4W_6' \right] \quad (21)$$

Bound energy calculated from (17), (20) and (18), (21) [21] related on global quantum number is shown in Table (see Table).

In result it was assumed that all particles' masses equal to the mass of electron. Parameter of correlation - $\gamma_i = 0.01$ ($i = 1, 2, 3$), the constants of interaction are the same, so $a_{ij} < 0$ and $b_{12} = b_{13} < 0$, $b_{23} > 0$, and various from 1 to 0.001 does not give qualitatively new results.

The results entered in table are true for a_{ij} in $(-1, -0.001)$ interval. Pair potential of the inverse square of the distance with repulsion interaction constants between particles (when $a_{ij} > 0$) was not considered in this paper and needs research in future. As regards to b_{ij} calculation had been made in case when they change according with modules in $(1; 0.001)$ interval and satisfy the conditions: $b_{12} = b_{13}$

< 0 , $b_{23} > 0$. For other values are not studied and needs research in future too.

Dependence of the bound state energy of three particle system on N - global quantum number for (14) pair potential

N	2D space		3D space	
	-E(compar.unit) formula (17)	-E (compar.unit) formula (20)	-E(compar.unit) formula (17)	-E(compar.unit) formula (21)
0	4.866238	4.7093248	0.3156439	0.304168
1	2.415242	2.3599785	0.1264723	0.123532
2	1.439093	1.413575	0.067679	0.066523
3	0.954168	0.9403576	0.042062	0.041494
4	0.678661	0.6703626	0.0286507	0.028331
5	0.507292	0.5019224	0.0207633	0.020566
6	0.393497	0.3898247	0.0157354	0.015605
7	0.314101	0.3114802	0.0123351	0.012244
8	0.256518	0.2545822	0.0099287	0.009863

Results obtained by calculation let us think that Schrödinger equation with (16) potential does not change its character by using MFHM. However, it can be used for the Schrödinger equation of three particle system for (16) pair interaction and not for (1) interaction. So we can give the answer to the equation in chapter two: 1) yes, only for (16) potential when a_{ij} is changing in $(-1; -0.001)$ interval and satisfied $b_{12} = b_{13} < 0$, $b_{23} > 0$ condition; 2) no, for (1) potential. So the values of bound state energy of three particle system when we used MFHM is real and has physical meaning only for (16) potentials.

4 CONCLUSIONS

The solution of three particles system of Schrödinger equation has given the following results:

1) Similar to (16) expression the pair interaction between the particles with MHFM and without MHFM (in first approximation) show that the binding energy of system dependence on the global quantum number in both cases are equal with grant precision (therefore MHFM does not change quality of Schrödinger equation)

when a_{ij} coefficients change interval is $(-1; -0.001)$ and b_{ij} coefficients change interval is $(1; 0.001)$ with condition $b_{12} = b_{13} < 0$, $b_{23} > 0$;

2) In order to obtain physically meaningful solution MFHM is applied for only two types of pair potentials: I. Critically singular potential; II. The sum of critically singular and Coulomb like potentials.

We have obtained that the calculated binding energy monotonously depends on the global quantum number.

3) By similar to (16) pair interaction between particles studied using MFHM in 2D and 3D spaces it was shown that with application of MFHM the solution of Schrödinger equation containing corresponding Hamiltonian to obtain the solution with physical meaning is possible.

4) By similar to (1) pair interaction between particles studied by MFHM in 2D and 3D spaces it was shown that solution of Schrödinger equation containing Hamiltonian is possible, but during solution there appears a component similar to Coulomb potential. Hence, we should not think that the obtained results correspond to the initially given investigated system (only to inverse square distance dependent pair potential three-particle system).

5. APPENDIX

Jo included in conditions (7) and (8) (similar to those obtained for (18) and (19)) represents the following expression:

$$J_o = \frac{\sqrt{3}}{2} (a_{12}J_{12} + a_{13}J_{13} + a_{23}J_{23}). \quad (d1)$$

As for J_{12} , (the analogous form have the others) it equals to:

$$J_{12} = \int \Phi_K^*(\Omega) \Phi_K(\Omega) (\cos \alpha)^{-2} d\Omega, \quad (d2)$$

where

$$\begin{aligned} \Phi_K(\Omega) = \\ = N_K^{l_1, l_2} \cos^{l_1} \alpha \sin^{l_2} \alpha P_n^{l_1+1/2, l_2+1/2}(\cos 2\alpha) Y_{l_1 m_1}(x) Y_{l_1 m_1}(y) \end{aligned} \quad (d3)$$

$P_n^{l_1+1, l_2+1}(\cos 2\alpha)$ – Jacob polynomial; $Y_{l_1 m_1}(x)$ – spherical function;

$$N_K^{l_1, l_2} = \left(\frac{2n!(K+2)(n+l_1+l_2+1)!}{\Gamma(n+l_1+3/2)\Gamma(n+l_2+3/2)} \right)^{1/2}; \quad n = \frac{K-l_1-l_2}{2}$$

putting (d3) in (d2), and taking into account that the work considers only the first approximation ($K = K' = 0$, $l_1 = l'_1 = l_2 = l'_2 = 0$), some transformations give:

$$J_{12} = \left(\frac{20!21!}{\Gamma(3/2)\Gamma(3/2)} \right) \left[\frac{\Gamma(3/2)}{\Gamma(1)\Gamma(3/2)} \frac{\Gamma(3/2)}{\Gamma(1)\Gamma(3/2)} \right]^2$$

$$2^0 (-1)^2 \frac{1}{2} \frac{\Gamma(3/2)\Gamma(1/2)}{\Gamma(2)} \quad (d4)$$

(d4) shows that, $J_{12} > 0$ (J_{13} and J_{14} are analogous). It follows from the (d1) J_0 sign depends on the sign of constants of interaction between panicles. In the paper only the case, when constant of interaction $a_{ij} < 0$ is considered, which notes that the work considers the case $J_0 < 0$.

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ა. ლომიძე

მანძილის კვადრატის უკუპროპორციული წყვილური პოტენციალის შემცველი სამნაწილაკოვანი სისტემის შრედინგერის განტოლების ამოხსნის ერთ-ერთი გზის შესახებ

მანძილის კვადრატის უკუპროპორციული წყვილური პოტენციალის მქონე სამნაწილაკოვანი სისტემის შრედინგერის განტოლების ამოხსნა აჩვენებს, რომ ბმული მდგომარეობა საერთოდ არ ხორციელდება ან ძირითადი მდგომარეობის ენერგია ტოლია - ∞ , რაც ფიზიკურად უაზროა. ამის მიზეზი არის ის, რომ პოტენციალი კრიტიკულად სინგულარულია [1-3].

ნაშრომი შეისწავლის მანძილის კვადრატის უკუპროპორციული წყვილური პოტენციალის შემცველი შრედინგერის განტოლების ამოხსნას პიპერსფერული ფუნქციის მოდიფიცირებული მეთოდის (მჰფმ) გამოყენებით [4-6], რომლის სარგებლობითაც შრედინგერის განტოლების შესაბამისი ჰამილტონიანი შეიცავს კრიტიკულად სინგულარულ პოტენციალთან ერთად კულონურის მსგავს პოტენციალს. ასეთი პოტენციალის შემცველი შრედინგერის განტოლების ამოხსნა შესაბამისი სასაზღვრო პირობებით მოცემულია კვანტური მექანიკის ნებისმიერ წიგნში და უშვებს ბმული სისტემის არსებობას. ნაშრომში ეს ამოხსნა იძლევა ზუსტ ფიზიკურ შედეგს და მიიღება, რომ პირველ მიახლოებაში სისტემის ბმის ენერგია იცვლება

მონოტონურად გლობალური კვანტური რიცხვის მიხედვით. თუმცა როგორც უკვე აღვნიშნეთ, ამ შემთხვევაში შესაბამის შრედინგერის განტოლებაში ჩნდება კულონური პოტენციალის მსგავსი წევრი, ამიტომ უნდა ვიფიქროთ, რომ მიღებული შედეგი არ შეესაბამება თავდაპირველად მოცემულ შესასწავლ სისტემას (მხოლოდ მანძილის კვადრატის უკუპროპორციული წყვილური პოტენციალის მქონე სამნაწილაკოვან სისტემას).