

States with non-zero angular momentum in the limit of large dimensionality

Contents

I. Introduction	1
II. One particle in a central field	2
A. S-states	2
B. Non-zero angular momentum states	3
III. Two particles in a central field	6
A. S-states	6
B. Non-zero angular momentum states	8
C. Inversion symmetry	10
D. Complete set of functions for a given angular momentum in $D \geq 4$	11
References	12

I. INTRODUCTION

Here, we consider a system of two particles bound in a central field. An example is a helium atom consisting of a heavy nucleus and two electrons. We generalize the problem to Cartesian space of D dimensions.

In D -dimensional Schrödinger equation, the number of arguments of the wave function grows as $2D$. For S-wave states the Schrödinger equation could be re-written in terms of only three “internal coordinates”, which are absolute values of vectors \mathbf{r}_1 , \mathbf{r}_2 , and the angle θ between them (instead of θ , one could alternatively use the inter-electron distance $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$). The dimensionality D enters as a parameter in the effective potential in this differential equation. This fact allows one to develop Rayleigh-Schrödinger perturbation

theory for small values of the parameter $1/D$. For the case of two-electron atoms, it leads to recurrence relations for coefficients of the series in $1/D$ [8–10].

In two extensive papers [5, 6] (more than 70 pages in total), Dunn and Watson factored out rotational degrees of freedom from internal degrees in the wave function of N particles bound in a central field. Their method is based on D -dimensional generalization of three-dimensional Schwartz expansion [14] (see also a simplified heuristic account of this work in [3]). In [4], Dunn and Watson showed that for the states with non-zero angular momentum of two-electron atoms, this approach reduces to solving of coupled differential equations in internal coordinates. In two subsequent papers [1, 7], Dunn and co-authors solved the resulting coupled equation in the large- D limit by developing a perturbation series in powers of $1/D$.

Dunn and Watson derived the coupled differential equations in internal coordinates using generalization of Wigner’s D -functions and sophisticated group-theoretical considerations. In current notes, we derive the same equations using a simplified approach based on purely algebraic manipulations.

For instructive purposes, we start from derivation of radial Schrödinger equation for one particle moving in a central field. Then, we generalize this approach to include a non-trivial case of two particles bound in a central field potential. Using symmetry of the wavefunction, we arrive finally to equations equivalent to those given by Dunn and Watson in [1].

II. ONE PARTICLE IN A CENTRAL FIELD

Schrödinger equation for a particle in a central potential $V(r)$ reads

$$-\frac{\nabla^2}{2}\Psi(\mathbf{r}) + V(r)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \quad (1)$$

where Ψ is the wavefunction, E is the energy, and we use atomic units, where the mass of the particle and Planck’s constant equal to one. We assume that $\mathbf{r} = (r^{(1)}, r^{(2)}, \dots, r^{(D)})$ is a vector in D -dimensional Cartesian space, and $r = |\mathbf{r}|$.

A. S-states

Let us consider a subspace of wavefunctions that have the following functional form

$$\Psi(\mathbf{r}) = \psi(r), \quad (2)$$

i.e. the functions of only one variable r .

The first derivative of (2) in respect to the i -th component of the radius-vector is

$$\frac{\partial}{\partial r^{(i)}} \Psi(\mathbf{r}) = \frac{r^{(i)}}{r} \psi'(r), \quad (3)$$

and the second derivative is

$$\frac{\partial^2}{\partial r^{(i)2}} \Psi(\mathbf{r}) = \frac{1}{r} \psi'(r) - \frac{r^{(i)2}}{r^3} \psi'(r) + \frac{r^{(i)2}}{r^2} \psi''(r). \quad (4)$$

Using equation (4), one could calculate the Laplacian as

$$\nabla^2 \Psi(\mathbf{r}) = \sum_{i=1}^D \frac{\partial^2}{\partial r^{(i)2}} \Psi(\mathbf{r}) = \psi''(r) + \frac{D-1}{r} \psi'(r). \quad (5)$$

Using equation (5), the original equation (1) in D coordinates reduces to a “radial” equation in only one variable r ,

$$[T_0 + V(r) - E] \psi(r) = 0, \quad (6)$$

where T_0 is the following differential operator

$$T_0 = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{D-1}{2r} \frac{d}{dr}. \quad (7)$$

Angular momentum could be generalized to D -dimensional space as a tensor whose components are operators

$$L_{i,j} = -i \left(r^{(i)} \frac{\partial}{\partial r^{(j)}} - r^{(j)} \frac{\partial}{\partial r^{(i)}} \right). \quad (8)$$

Since for the wavefunction of the form given by equation (2)

$$L_{i,j} \Psi(\mathbf{r}) = 0, \quad (9)$$

it could be considered as a generalization of S-state to D dimensions. Thus, we derive here radial Schrödinger equation for S-states by guessing their functional form.

B. Non-zero angular momentum states

Here, we assume that $D \geq 2$ and l is some non-negative integer. Let us consider a subspace of wavefunctions of the following functional form

$$\Psi(\mathbf{r}) = (x + iy)^l \psi(r), \quad x \equiv r^{(1)}, y \equiv r^{(2)}. \quad (10)$$

Since the case of $l = 0$ simply reduces to S-state wavefunctions given by equation (2), we assume henceforward that $l > 0$.

Laplacian of the function (10) is

$$\nabla^2 \Psi(\mathbf{r}) = [\nabla^2(x + iy)^l] \psi(r) + 2(\nabla(x + iy)^l, \nabla \psi(r)) + (x + iy)^l \nabla^2 \psi(r). \quad (11)$$

The first term in equation (11) is zero because $\nabla^2(x + iy)^l$. The second term is

$$2(\nabla(x + iy)^l, \nabla \psi(r)) = 2 \left(\frac{\partial}{\partial x}(x + iy)^l \right) \left(\frac{\partial}{\partial x} \psi(r) \right) + 2 \left(\frac{\partial}{\partial y}(x + iy)^l \right) \left(\frac{\partial}{\partial y} \psi(r) \right) = 2l \Psi(\mathbf{r}), \quad (12)$$

and the third term could be calculated in the same way as in Subsection II A,

$$(x + iy)^l \nabla^2 \psi(r) = (x + iy)^l \left(\psi''(r) + \frac{D-1}{r} \psi'(r) \right), \quad (13)$$

Using equations (12) and (13) and factoring out the term $(x + iy)^l$, we reduce the original Schrödinger equation (1) to the “radial” equation

$$(T_l + V(r) - E) \psi(r) = 0, \quad (14)$$

where T_l is the differential operator

$$T_l = T_0 - \frac{l}{r} \frac{d}{dr} = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{2l + D - 1}{2r} \frac{d}{dr}, \quad (15)$$

and T_0 is given by equation (7).

Now, let us calculate actions of different components of the tensor of angular momentum (8) on the wavefunction of the functional form given by equation (10). If $i = 1$ and $j = 2$, then

$$L_{1,2} \Psi(\mathbf{r}) = -ix \left[il(x + iy)^{l-1} \psi(r) + (x + iy)^l \frac{y}{r} \psi'(r) \right] + iy \left[l(x + iy)^{l-1} \psi(r) + (x + iy)^l \frac{x}{r} \psi'(r) \right]. \quad (16)$$

In equation (16), second and fourth terms cancel, and we have

$$L_{1,2} \Psi(\mathbf{r}) = l(x + iy)(x + iy)^{l-1} = l \Psi(\mathbf{r}). \quad (17)$$

If $j > 2$, then

$$L_{1,j} \Psi(\mathbf{r}) = ilr^{(j)}(x + iy)^{l-1} \psi(r), \quad L_{2,j} \Psi(\mathbf{r}) = -lr^{(j)}(x + iy)^{l-1} \psi(r). \quad (18)$$

Finally, if $i > 2$ and $j > 2$, then

$$L_{i,j}\Psi(\mathbf{r}) = 0. \quad (19)$$

We generalize rotationally-invariant square of angular momentum to D -dimensional space as

$$L^2 = \sum_{i < j} L_{i,j}^2. \quad (20)$$

Calculating action of operators $L_{i,j}^2$ on $\Psi(\mathbf{r})$, we find

$$L_{1,2}^2\Psi(\mathbf{r}) = l^2\Psi(\mathbf{r}), \quad (21a)$$

$$L_{1,j}^2\Psi(\mathbf{r}) = lx(x+iy)^{l-1}\psi(r) - l(l-1)r^{(j)2}(x+iy)^{l-2}\psi(r), \quad j > 2 \quad (21b)$$

$$L_{j,2}^2\Psi(\mathbf{r}) = l(l-1)r^{(j)2}(x+iy)^{l-2}\psi(r) + ily(x+iy)^{l-1}\psi(r), \quad j > 2 \quad (21c)$$

$$L_{i,j}^2\Psi(\mathbf{r}) = 0, \quad i > 2, j > 2. \quad (21d)$$

Using equations (21b) and (21c) we find

$$(L_{1,j}^2 + L_{j,2}^2)\Psi(\mathbf{r}) = l\Psi(\mathbf{r}), \quad j > 2. \quad (22)$$

Using equations (21a), (22), and (21d) we find

$$L^2\Psi(\mathbf{r}) = L_{1,2}^2\Psi(\mathbf{r}) + \sum_{j=3}^D (L_{1,j}^2\Psi(\mathbf{r}) + L_{j,2}^2\Psi(\mathbf{r})) + \sum_{3 \leq i < j \leq D} L_{i,j}^2\Psi(\mathbf{r}) = l(l+D-2)\Psi(\mathbf{r}). \quad (23)$$

Equation (23) means that the function $\Psi(\mathbf{r})$ is eigenfunction of square of angular momentum with non-zero eigenvalue. Thus, equation (14) represents radial equation for wavefunctions with a non-zero angular momentum.

Current approach is based on guessing right functional form of the wavefunction of non-zero angular momentum. Here, we chose only one particular functional form corresponding to one of many possible spacial orientations of the angular momentum. Determining and counting all independent functional forms is possible through l -th degree homogeneous harmonic polynomials (i.e. polynomials satisfying the Laplacian differential equation), see for example a textbook of Kramers[13]. Another possible eigenfunctions of L^2 include for example functions of the form $\left(\sum_{i=1}^D c_i r^{(i)}\right)^l \psi(r)$ where c_1, c_2, \dots, c_D are any constants satisfying equation $\sum_{i=1}^D c_i^2 = 0$. Kramers found the number of linearly independent functional forms in three-dimensional space to be $2l + 1$ by firstly counting the number of coefficients in the l -th degree homogeneous polynomial, $\frac{1}{2}(l+1)(l+2)$, and then subtracting the number of

constraints, $\frac{1}{2}l(l-1)$. By adjusting Kramer's argument to D -dimensional space, one could easily estimate the number of linearly independent functional forms in general case of D dimensions as

$$\frac{(2l+D-2)(l+D-3)!}{(D-2)!l!} = \frac{(l+D-1)!}{(D-1)!l!} - \frac{(l+D-3)!}{(D-1)!(l-2)!}. \quad (24)$$

Particularly for $D=2$, there are two independent functions $(x \pm iy)^l \psi(r)$ which obviously correspond to two possible eigenvalues $\pm l$ of $L_{1,2}$. It should be noted that the radial equation is the same for all functions with the given eigenvalue of L^2 , but the orientations of the angular momentum in space are different.

III. TWO PARTICLES IN A CENTRAL FIELD

Schrödinger equation for two particles in a central field reads

$$\left[-\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} + V(r_1, r_2, r_{12}) - E \right] \Psi(\mathbf{r}_1, \mathbf{r}_2) = 0, \quad (25)$$

where Ψ is the wavefunction, E is the energy, V is the potential of interaction of the particles with the central field plus the potential of interaction between the particles, and we use units, where the mass of each particle and Planck's constant equal to one. We assume that $r_1 = |\mathbf{r}_1|$, $r_2 = |\mathbf{r}_2|$, and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. Everywhere in this section we use the same notations as those for the case of one particle in Section II, but now the potential and the wavefunction have larger number of arguments.

A. S-states

Let us consider a subspace of wavefunctions that have the following functional form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(r_1, r_2, r_{12}), \quad (26)$$

i.e. the functions of only three variables r_1, r_2, r_{12} . The following derivations are completely analogous to those in Subsection II A for the case of one particle.

First derivatives of (26) in respect to the i -th component of \mathbf{r}_1 and \mathbf{r}_2 are

$$\begin{aligned} \frac{\partial}{\partial r_1^{(i)}} \Psi(\mathbf{r}_1, \mathbf{r}_2) &= \frac{r_1^{(i)}}{r_1} \psi'_{r_1}(r_1, r_2, r_{12}) + \frac{r_1^{(i)} - r_2^{(i)}}{r_{12}} \psi'_{r_{12}}(r_1, r_2, r_{12}), \\ \frac{\partial}{\partial r_2^{(i)}} \Psi(\mathbf{r}_1, \mathbf{r}_2) &= \frac{r_2^{(i)}}{r_2} \psi'_{r_2}(r_1, r_2, r_{12}) + \frac{r_2^{(i)} - r_1^{(i)}}{r_{12}} \psi'_{r_{12}}(r_1, r_2, r_{12}), \end{aligned} \quad (27)$$

and second derivatives are

$$\begin{aligned}
\frac{\partial^2}{\partial r_1^{(i)2}} \Psi(\mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{r_1} \psi'_{r_1}(r_1, r_2, r_{12}) - \frac{r_1^{(i)2}}{r_1^3} \psi'_{r_1}(r_1, r_2, r_{12}) + \frac{r_1^{(i)2}}{r_1^2} \psi''_{r_1, r_1}(r_1, r_2, r_{12}) \\
&+ \frac{1}{r_{12}} \psi'_{r_{12}}(r_1, r_2, r_{12}) - \frac{(r_1^{(i)} - r_2^{(i)})^2}{r_{12}^3} \psi'_{r_{12}}(r_1, r_2, r_{12}) \\
&+ \frac{(r_1^{(i)} - r_2^{(i)})^2}{r_{12}^2} \psi''_{r_{12}, r_{12}}(r_1, r_2, r_{12}) + 2 \frac{r_1^{(i)}(r_1^{(i)} - r_2^{(i)})}{r_1 r_{12}} \psi''_{r_1, r_{12}}(r_1, r_2, r_{12}),
\end{aligned} \tag{28a}$$

$$\begin{aligned}
\frac{\partial^2}{\partial r_2^{(i)2}} \Psi(\mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{r_2} \psi'_{r_2}(r_1, r_2, r_{12}) - \frac{r_2^{(i)2}}{r_2^3} \psi'_{r_2}(r_1, r_2, r_{12}) + \frac{r_2^{(i)2}}{r_2^2} \psi''_{r_2, r_2}(r_1, r_2, r_{12}) \\
&+ \frac{1}{r_{12}} \psi'_{r_{12}}(r_1, r_2, r_{12}) - \frac{(r_2^{(i)} - r_1^{(i)})^2}{r_{12}^3} \psi'_{r_{12}}(r_1, r_2, r_{12}) \\
&+ \frac{(r_2^{(i)} - r_1^{(i)})^2}{r_{12}^2} \psi''_{r_{12}, r_{12}}(r_1, r_2, r_{12}) + 2 \frac{r_2^{(i)}(r_2^{(i)} - r_1^{(i)})}{r_2 r_{12}} \psi''_{r_2, r_{12}}(r_1, r_2, r_{12}).
\end{aligned} \tag{28b}$$

Using equations (28a) and (28b), one could calculate

$$\begin{aligned}
(\nabla_1^2 + \nabla_2^2) \Psi(\mathbf{r}_1, \mathbf{r}_2) &= \sum_{i=1}^D \left(\frac{\partial^2}{\partial r_1^{(i)2}} + \frac{\partial^2}{\partial r_2^{(i)2}} \right) \Psi(\mathbf{r}_1, \mathbf{r}_2) \\
&= \psi''_{r_1, r_1}(r_1, r_2, r_{12}) + \psi''_{r_2, r_2}(r_1, r_2, r_{12}) + 2 \psi''_{r_{12}, r_{12}}(r_1, r_2, r_{12}) \\
&+ \frac{r_{12}^2 + r_1^2 - r_2^2}{r_1 r_{12}} \psi''_{r_1, r_{12}}(r_1, r_2, r_{12}) + \frac{r_{12}^2 + r_2^2 - r_1^2}{r_2 r_{12}} \psi''_{r_2, r_{12}}(r_1, r_2, r_{12})
\end{aligned} \tag{29}$$

Using equation (29), equation (25) reduces to an equation in “internal” coordinates r_1, r_2, r_{12} ,

$$[T + V(r_1, r_2, r_{12}) - E] \psi(r_1, r_2, r_{12}) = 0, \tag{30}$$

where T is the differential operator

$$\begin{aligned}
T &= -\frac{1}{2} \left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + 2 \frac{\partial^2}{\partial r_{12}^2} \right. \\
&+ 2 \frac{r_1^2 + r_{12}^2 - r_2^2}{r_1 r_{12}} \frac{\partial^2}{\partial r_1 \partial r_{12}} + 2 \frac{r_2^2 + r_{12}^2 - r_1^2}{r_2 r_{12}} \frac{\partial^2}{\partial r_2 \partial r_{12}} \\
&\left. + \frac{D-1}{r_1} \frac{\partial}{\partial r_1} + \frac{D-1}{r_2} \frac{\partial}{\partial r_2} + 2 \frac{D-1}{r_{12}} \frac{\partial}{\partial r_{12}} \right).
\end{aligned} \tag{31}$$

(i, j) -component of the operator of total angular momentum is

$$L_{i,j} = -i \left(r_1^{(i)} \frac{\partial}{\partial r_1^{(j)}} - r_1^{(j)} \frac{\partial}{\partial r_1^{(i)}} + r_2^{(i)} \frac{\partial}{\partial r_2^{(j)}} - r_2^{(j)} \frac{\partial}{\partial r_2^{(i)}} \right). \tag{32}$$

Since for the wavefunction of the form given by equation (26)

$$L_{i,j}\Psi(\mathbf{r}_1, \mathbf{r}_2) = 0, \quad (33)$$

it describes S-state.

B. Non-zero angular momentum states

Assuming that $D \geq 2$ and $l > 0$ is an integer, we consider a subspace of wavefunctions of the following functional form

$$\Psi_l(\mathbf{r}_1, \mathbf{r}_2) = \sum (x_1 + iy_1)^{l_1} (x_2 + iy_2)^{l_2} \psi^{(l_1, l_2)}(r_1, r_2, r_{12}), \quad (34)$$

where summation is performed for all possible non-negative integer numbers l_1, l_2 satisfying equation

$$l_1 + l_2 = l \quad (35)$$

and

$$x_1 \equiv r_1^{(1)}, y_1 \equiv r_1^{(2)}, x_2 \equiv r_2^{(1)}, y_2 \equiv r_2^{(2)}. \quad (36)$$

Taking into account that $\nabla_1(x_1 + iy_1)^{l_1} = 0$, $\nabla_2(x_2 + iy_2)^{l_2} = 0$ and that $-1/2(\nabla_1^2 + \nabla_2^2)\psi^{(l_1, l_2)}(r_1, r_2, r_{12}) = T\psi^{(l_1, l_2)}(r_1, r_2, r_{12})$ where T is the differential operator given by equation (31), we could calculate the kinetic energy term as

$$\begin{aligned} \left(-\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2}\right) \Psi(\mathbf{r}_1, \mathbf{r}_2) &= \sum \left\{ (x_1 + iy_1)^{l_1} (x_2 + iy_2)^{l_2} T\psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right. \\ &\quad - (x_2 + iy_2)^{l_2} \left([\nabla_1(x_1 + iy_1)^{l_1}], \nabla_1\psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right) \\ &\quad \left. - (x_1 + iy_1)^{l_1} \left([\nabla_2(x_2 + iy_2)^{l_2}], \nabla_2\psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right) \right\} \end{aligned} \quad (37)$$

The second term in the sum in r.h.s of equation (37) is

$$\begin{aligned}
& -(x_2 + iy_2)^{l_2} \left([\nabla_1(x_1 + iy_1)^{l_1}], \nabla_1 \psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right) = \\
& - (x_2 + iy_2)^{l_2} \left[\left(\frac{\partial}{\partial x_1} (x_1 + iy_1)^{l_1} \right) \left(\frac{\partial}{\partial x_1} \psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right) \right. \\
& \left. + \left(\frac{\partial}{\partial y_1} (x_1 + iy_1)^{l_1} \right) \left(\frac{\partial}{\partial y_1} \psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right) \right] = \\
& - (x_2 + iy_2)^{l_2} l_1 (x_1 + iy_1)^{l_1-1} \left[\left(\frac{x_1}{r_1} + i \frac{y_1}{r_1} \right) \psi'_{r_1}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) \right. \\
& \left. + \left(\frac{x_1 - x_2}{r_{12}} + i \frac{y_1 - y_2}{r_{12}} \right) \psi'_{r_{12}}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) \right] = \\
& - l_1 (x_1 + iy_1)^{l_1} (x_2 + iy_2)^{l_2} \left[\frac{1}{r_1} \psi'_{r_1}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) + \frac{1}{r_{12}} \psi'_{r_{12}}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) \right] \\
& + l_1 (x_1 + iy_1)^{l_1-1} (x_2 + iy_2)^{l_2+1} \left[\frac{1}{r_{12}} \psi'_{r_{12}}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) \right], \tag{38}
\end{aligned}$$

where we used formulas for derivatives given by equation (27).

The third term in the sum in r.h.s of equation (37) could be calculated in the same way as in equation (38),

$$\begin{aligned}
& -(x_1 + iy_1)^{l_1} \left([\nabla_2(x_2 + iy_2)^{l_2}], \nabla_2 \psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right) = \\
& - l_2 (x_1 + iy_1)^{l_1} (x_2 + iy_2)^{l_2} \left[\frac{1}{r_2} \psi'_{r_2}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) + \frac{1}{r_{12}} \psi'_{r_{12}}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) \right] \\
& + l_2 (x_1 + iy_1)^{l_1+1} (x_2 + iy_2)^{l_2-1} \left[\frac{1}{r_{12}} \psi'_{r_{12}}{}^{(l_1, l_2)}(r_1, r_2, r_{12}) \right]. \tag{39}
\end{aligned}$$

Finally, combining equations (37), (38), (39) we obtain

$$\begin{aligned}
& \left(-\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} \right) \Psi(\mathbf{r}_1, \mathbf{r}_2) \\
& = \sum \left\{ (x_1 + iy_1)^{l_1} (x_2 + iy_2)^{l_2} \left(T - \frac{l_1}{r_1} \frac{\partial}{\partial r_1} - \frac{l_2}{r_2} \frac{\partial}{\partial r_2} - \frac{l}{r_{12}} \frac{\partial}{\partial r_{12}} \right) \psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right. \\
& \left. - [l_1 (x_1 + iy_1)^{l_1-1} (x_2 + iy_2)^{l_2+1} + l_2 (x_1 + iy_1)^{l_1+1} (x_2 + iy_2)^{l_2-1}] \frac{1}{r_{12}} \frac{\partial}{\partial r_{12}} \psi^{(l_1, l_2)}(r_1, r_2, r_{12}) \right\}. \tag{40}
\end{aligned}$$

Let us define $l + 1$ -component vector ψ as

$$\psi(r_1, r_2, r_{12}) = (\psi^{(0, l)}(r_1, r_2, r_{12}), \psi^{(1, l-1)}(r_1, r_2, r_{12}), \dots, \psi^{(l, 0)}(r_1, r_2, r_{12})) \tag{41}$$

and $(l + 1) \times (l + 1)$ matrices \mathbf{I} , \mathbf{A}^+ , \mathbf{A}^- , \mathbf{B}^+ , \mathbf{B}^- as

$$\begin{aligned}
I_{l_1, l_2} &= \delta_{l_1, l_2}, \\
A_{l_1, l_2}^+ &= l_1 \delta_{l_1, l_2}, \\
A_{l_1, l_2}^- &= l_2 \delta_{l_1, l_2}, \\
B_{l_1, l_2}^+ &= l_1 \delta_{l_1-1, l_2}, \\
B_{l_1, l_2}^- &= l_2 \delta_{l_1, l_2-1}.
\end{aligned} \tag{42}$$

Then, taking into account equation (40) we could see that the Schrödinger equation (25) is satisfied if the following system of $l + 1$ differential equations written in a vector form holds,

$$\left[\left(T - \frac{l}{r_{12}} \frac{\partial}{\partial r_{12}} + V(r_1, r_2, r_{12}) - E \right) \mathbf{I} - \frac{1}{r_1} \frac{\partial}{\partial r_1} \mathbf{A}^+ - \frac{1}{r_2} \frac{\partial}{\partial r_2} \mathbf{A}^- - \frac{1}{r_{12}} \frac{\partial}{\partial r_{12}} (\mathbf{B}^+ + \mathbf{B}^-) \right] \psi = 0. \tag{43}$$

C. Inversion symmetry

Since the potential does not change under the transformation of inversion, $\mathbf{r}_1 \rightarrow -\mathbf{r}_1$, $\mathbf{r}_2 \rightarrow -\mathbf{r}_2$, the wavefunction should have certain parity $\pi = \pm 1$, i.e. either it does not change under inversion or it is multiplied by (-1) . For the particular chosen functional form (34), the parity is determined through l as $\pi = (-1)^l$. It is easy to see that equation (43) is identical to the formula (4) from the paper [1] with their $x = L$ equal to our l and their matrices \mathbf{L}_x and \mathbf{S}_x related to our matrices (42) as $\frac{1}{2}(\mathbf{L}_x \pm \mathbf{L}_x) = \mathbf{A}^\pm$, $\mathbf{S}_x = \mathbf{B}^+ + \mathbf{B}^-$. There should be taken into account two misprints in their formula (4), $+\mathbf{L}_x \rightarrow -\mathbf{L}_x$ in 5-th line and $2r_{12} \rightarrow r_{12}$ in a denominator of the last line (the misprints could be spotted by comparison of the formula (4) with a similar formula (24) from their earlier paper [4]).

Since the function (34) for a given l has only one possible parity, this functional form does not span all possible symmetries. In one of the earliest papers about dimensionality dilation and its use in atomic physics, Herrick and Stillinger [12] proved that some of P-states of helium atom have the same energy as S-states, but in a non-physical 5-dimensional space. There, he used the following functional form for the wave function,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = (x_1 y_2 - x_2 y_1) \psi(r_1, r_1, r_{12}), \tag{44}$$

where x_i and y_i are the first and the second coordinates of i -th electron ($i = 1, 2$). This fact

provides a hint to try a more general functional form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = (x_1 y_2 - x_2 y_1) \sum (x_1 + i y_1)^{l_1} (x_2 + i y_2)^{l_2} \psi^{(l_1, l_2)}(r_1, r_2, r_{12}), \quad (45)$$

where summation is performed for all possible non-negative integer numbers l_1, l_2 satisfying equation

$$l_1 + l_2 = l - 1 \quad (46)$$

for a given positive integer l . However, this naive attempt fails. Let us consider 2-dimensional space. Then, there is only one component of angular momentum $L_{1,2}$ whose eigenvalues are integer numbers $\pm l$. Since the operation of inversion in a plane could be expressed through $L_{1,2}$ as $\exp(i\pi L_{1,2})$, the function of angular momentum l has always a certain parity $\exp(i\pi l) = (-1)^l$. Therefore, functions that have an opposite parity $(-1)^{l+1}$ in two dimensions simply does not exist!

Duan and co-authors [2] gave a formula for states of two possible parity in three dimensions. This functional form could be equally used in any dimensionality $D \geq 3$,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = [(x_1 + i y_1) z_2 - (x_2 + i y_2) z_1] \sum_{l_1 + l_2 = l - 1} (x_1 + i y_1)^{l_1} (x_2 + i y_2)^{l_2} \psi^{(l_1, l_2)}(r_1, r_2, r_{12}), \quad (47)$$

where z_i is the third coordinate of i -th electron. The wavefunction given by equation (47) is complementary to the wavefunction given by equation (34) in a sense that while the former has parity $-(-1)^l$, the latter has parity $(-1)^l$. It could be proven by direct calculations that the differential equations for l functions $\psi^{(l_1, l_2)}(r_1, r_2, r_{12})$ are given by old formula (43) in which D (in a definition of the operator T) is replaced by $D+2$ and l is replaced by $l-1$. This formula is identical to the formula (4) from the paper [1] with their $x = L - 1$ equal to our $l-1$. Since equations are the same both for $(D, l, \pi = (-1)^l)$ and for $(D+2, l-1, \pi = -(-1)^l)$ states, the energies are equal (“interdimensional degeneracies”).

D. Complete set of functions for a given angular momentum in $D \geq 4$

As it was stated in [2], wavefunctions given by equations (34) and (47) constitute a complete set for the given angular momentum in three dimensions. Later, Gu and co-authors generalized their approach to the space of D dimensions [11]. It appears that there exist even more general functions of a given angular momentum in the space of dimensionality

$D \geq 4$,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = [(x_1 + iy_1)(z_2 + iw_2) - (x_2 + iy_2)(z_1 + iw_1)]^\nu \times \sum_{l_1+l_2=l-\nu} (x_1 + iy_1)^{l_1} (x_2 + iy_2)^{l_2} \psi^{(l_1, l_2)}(r_1, r_2, r_{12}), \quad (48)$$

where w_i is the fourth coordinate of i -th electron, and ν is an integer $0 \leq \nu \leq l$. In a particular case of $\nu = 0$, equation (48) is equivalent to equation (34). In case of $\nu = 1$, it has a slightly different form from equation (47) (because of presence of coordinates w_1 and w_2), but the equation for radial functions $\psi^{(l_1, l_2)}(r_1, r_2, r_{12})$ remain the same (compare with the same fact for P-functions $x\psi(r)$ and $(x + iy)\psi(r)$ in case of one particle). The set of differential equations for $l - \nu + 1$ functions $\psi^{(l_1, l_2)}(r_1, r_2, r_{12})$ are given by old formula (43) in which D is replaced by $D + 2\nu$ and l is replaced by $l - \nu$. Thus (D, l, ν) and $(D - 2, l + 1, \nu + 1)$ states have always the same energy yielding the complete spectrum of “interdimensional degeneracies” [11]. This fact effectively reduces any state in even dimensionality larger than 4 to some $l \neq 0$ state in four dimensions and any state in odd dimensionality larger than 4 to some $l \neq 0$ state in $D = 5$.

-
- [1] J. C. Carzoli, M. Dunn, and D. K. Watson, *Singly and doubly excited states of the D -dimensional helium atom*, Phys. Rev. A **59** (1999), 182–187.
- [2] B. Duan, X.-Y. Gu, and Z.-Q. Ma, *Precise calculation for energy levels of a helium atom in P states*, Physics Letters A **283** (2001), 229–236.
- [3] M. Dunn and D. K. Watson, *Analytical continuation of higher angular momentum states to D dimensions and interdimensional degeneracies*, Dimensional Scaling in Chemical Physics (D. R. Herschbach, J. Avery, and O. Goscinski, eds.), Kluwer Academic, Dordrecht, 1993, pp. 375–388.
- [4] ———, *Continuation of the Schrödinger Equation for Higher Angular-Momentum States to D Dimensions and Interdimensional Degeneracies*, Few-Body Syst. **21** (1996), 187–209.
- [5] ———, *Continuation of the Wave Function for Higher Angular Momentum States to D Dimensions. I. The Generalized Schwartz Expansion*, Ann. Phys. (N. Y.) **251** (1996), 266–318.
- [6] ———, *Continuation of the Wave Function for Higher Angular Momentum States to D Dimensions. II. Elimination of Linear Dependencies*, Ann. Phys. (N. Y.) **251** (1996), 319–

336.

- [7] ———, *Large-dimension limit of higher-angular-momentum states of two-electron atoms*, Phys. Rev. A **59** (1999), 1109–1124.
- [8] D. Z. Goodson and D. R. Herschbach, *Recursive calculation of dimensional expansions for two-electron atoms*, Phys. Rev. Lett. **58** (1987), 1628–1631.
- [9] D. Z. Goodson, M. López-Cabrera, D. R. Herschbach, and J. D. Morgan, III, *Large-order dimensional perturbation theory for two-electron atoms*, J. Chem. Phys. **97** (1992), 8481–8496.
- [10] D. Z. Goodson and D. K. Watson, *Dimensional perturbation theory for excited states of two-electron atoms*, Phys. Rev. A **48** (1993), 2668–2678.
- [11] X.-Y. Gu, Z.-Q. Ma, and B. Duan, *Interdimensional degeneracies for a quantum three-body system in D dimensions*, Physics Letters A **307** (2003), 55–59.
- [12] D. R. Herrick and F. H. Stillinger, *Variable dimensionality in atoms and its effect on the ground state of the helium isoelectronic sequence*, Phys. Rev. A **11** (1975), 42–53.
- [13] H. A. Kramers, *Quantum mechanics*, Courier Dover Publications, 2003.
- [14] C. Schwartz, *Lamb Shift in the Helium Atom*, Phys. Rev. **123** (1961), 1700–1705.