Bohr orbits in space of many dimensions

For systems like a particle moving in central field, there exists a state of the lowest energy for any given non-zero angular momentum. These lowest-energy states are commonly known as circular states in quantum mechanics or as Bohr orbits in classical mechanics. The concept of Bohr orbits is generalized for any number of particles moving in central field in space of D Cartesian coordinates. Bohr orbit for two particles is explicitly constructed.

I. DEFINITION OF BOHR ORBIT FOR N ELECTRONS IN D-DIMENSIONAL SPACE

A. $N = 1$, $D = 3$

Normally, Bohr orbit is defined for a single electron ($N = 1$) moving in a central field of a nucleus in the physical three-dimensional space. It may be considered as a classical analogue of a quantum mechanical ground state, i.e. the state of the lowest energy for a given angular momentum.

For a given value of L, a trajectory of classical motion could be easily found by separating angular and radial motions. Then, the motion in radial coordinate r reduces to the motion in an effective potential $V(r) + L^2/(2r^2)$. Classically, any energies are allowed as long as E is greater than the minimum of the effective potential, $E \geq V_{\min}$. The Bohr orbit appears in the extreme limit of $E = V_{\min}$, which obviously corresponds to a circular motion with a constant r.

From a formal point of view, there is a unique Bohr orbit for any vector of angular momentum, except zero angular momentum, when the effective potential has no minimum, and the state "collapses" to the nucleus.

B. Generalization to arbitrary D and N

In a space of arbitrary dimensionality D, an angular momentum is characterized by a tensor L which is described in a given basis set by an antisymmetric matrix

$$\mathcal{L}_{ij} = \sum_{n=1}^{N} \left(r_i^{(n)} p_j^{(n)} - r_j^{(n)} p_i^{(n)} \right) . \tag{1}$$

For any given antisymmetric matrix $\{L_{ij}\}$, there could be three possibilities.

(1) No classical motion exists for which $\mathcal{L}_{ij} = L_{ij}$, where $\mathcal{L}_{ij}$ is given by equation (1). It occurs for example for one electron in four-dimensional space for the matrix given by equation (2), see the proof in Section II C.

(2) There exists a classical motion for which $\mathcal{L}_{ij} = L_{ij}$ for **any** energy, i.e. there is no minimal energy. It occurs for example for two electrons in three-dimensional space, when one electron could "collapse" to the nucleus, while the second electron could carry the required angular momentum.

(3) There is a minimal energy $E_{\min}$, so that a classical motion for which $\mathcal{L}_{ij} = L_{ij}$ exists if and only if $E \geq E_{\min}$.

In the latter case, we call **Bohr orbit** or **Bohr motion** the classical motion with $\mathcal{L}_{ij} = L_{ij}$ and with the minimal energy, $E = E_{\min}$.

II. NON-TRIVIAL EXAMPLE OF BOHR ORBIT: TWO ELECTRONS IN FOUR-DIMENSIONAL SPACE

As it was mentioned above in section I B, Bohr orbits do not exist for two electrons in three-dimensional space for any angular momentum because of the effect of "collapse" of one or both electrons (if $L \neq 0$ or $L = 0$ respectively). Here, we show that in **four** dimensional space ($D = 4$), Bohr orbits exist at least for some angular momenta.

Consider, for example the antisymmetric matrix

$$\mathsf{L} = \begin{pmatrix} 0 & \lambda & 0 & 0 \\ -\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda \\ 0 & 0 & -\lambda & 0 \end{pmatrix} \tag{2}$$

whose only non-zero elements are $L_{12} = -L_{21} = L_{34} = -L_{43} = \lambda$ (we assume here that $\lambda \neq 0$).

The Hamiltonian of a four-dimensional helium is

$$H = T + V, \tag{3}$$

where

$$T = \frac{1}{2}\left(\boldsymbol{p}^2 + \boldsymbol{q}^2\right), \quad V = -\frac{2}{|\boldsymbol{r}|} - \frac{2}{|\boldsymbol{s}|} + \frac{2}{|\boldsymbol{r} - \boldsymbol{s}|}, \tag{4}$$

where $\boldsymbol{p} \equiv \boldsymbol{p}^{(1)}$, $\boldsymbol{q} \equiv \boldsymbol{p}^{(2)}$, $\boldsymbol{r} \equiv \boldsymbol{r}^{(1)}$, $\boldsymbol{s} \equiv \boldsymbol{r}^{(2)}$.

Here, we impose six constraints demanding that the tensor of angular momentum be equal to that of equation (2),

$$L_{12} = r_1p_2 - r_2p_1 + s_1q_2 - s_2q_1 = \lambda, \tag{5}$$

$$L_{34} = r_3p_4 - r_4p_3 + s_3q_4 - s_4q_3 = \lambda, \tag{6}$$

$$L_{13} = r_1p_3 - r_3p_1 + s_1q_3 - s_3q_1 = 0, \tag{7}$$

$$L_{24} = r_2p_4 - r_4p_2 + s_2q_4 - s_4q_2 = 0, \tag{8}$$

$$L_{14} = r_1p_4 - r_4p_1 + s_1q_4 - s_4q_1 = 0, \tag{9}$$

$$L_{23} = r_2p_3 - r_3p_2 + s_2q_3 - s_3q_2 = 0. \tag{10}$$

Minimization of the Hamiltonian as a function of sixteen variables (eight coordinates and eight momenta) with constraints (5) - (10) was done numerically for $\lambda = 1$ using Mathematica software, that gives the minimal energy $E_{\min} = -2.73777$ which is exactly the same as a quantum-mechanical energy in the infinite-D limit.

A. Analytic minimization

Minimization is hard to be done analytically without further simplifications. As it will be shown in Subsection II B, under an appropriate choice of coordinate system the matrix L remains the same as given by equation (2), while vectors of coordinates $\boldsymbol{r}$ and $\boldsymbol{s}$ lie in $(1,3)$ plane, i.e.

$$r_2 = r_4 = s_2 = s_4 = 0. \tag{11}$$

Here, we use such a basis set in order to simplify the equations.

Among the equations (5) - (10), equation (7) will be automatically satisfied, while equation (8) remains unchanged. Other four equations, (5), (6), (9), (10) may be used to express momenta p_2, q_2, p_4, and q_4 through coordinates and subtitute them into the kinetic energy.

Taking into account (11), equations (5) and (10) are rewritten as

$$r_1 p_2 + s_1 q_2 = \lambda, \tag{12}$$

$$-r_3 p_2 - s_3 q_2 = 0. \tag{13}$$

Solving equations (12) and (13) in respect to p_2 and q_2, we obtain

$$p_2 = -\frac{\lambda s_3}{r_3 s_1 - r_1 s_3}, \tag{14}$$

$$q_2 = \frac{\lambda r_3}{r_3 s_1 - r_1 s_3}. \tag{15}$$

In a similar way, equations (6) and (9) are rewritten as

$$r_3 p_4 + s_3 q_4 = \lambda, \tag{16}$$

$$r_1 p_4 + s_1 q_4 = 0. \tag{17}$$

Solving equations (16) and (17) in respect to p_4 and q_4, we obtain

$$p_4 = \frac{\lambda s_1}{r_3 s_1 - r_1 s_3}, \tag{18}$$

$$q_4 = -\frac{\lambda r_1}{r_3 s_1 - r_1 s_3}. \tag{19}$$

Now, substituting the momenta given by equations (14), (15), (18), (19) into the kinetic energy $T = \frac{1}{2}(p_1^2 + p_2^2 + p_3^2 + p_4^2 + q_1^2 + q_2^2 + q_3^2 + q_4^2)$, we obtain,

$$T = \frac{1}{2}(p_1^2 + p_3^2 + q_1^2 + q_3^2) + V_{\mathrm{c}}(\boldsymbol{r}, \boldsymbol{s}), \tag{20}$$

where V_{c} is an analogue of a centrifugal energy,

$$V_{\mathrm{c}}(\boldsymbol{r}, \boldsymbol{s}) = \frac{\lambda^2}{2} \frac{(r_1^2 + r_3^2 + s_1^2 + s_3^2)}{(r_3 s_1 - r_1 s_3)^2}. \tag{21}$$

Noticing that $(r_3 s_1 - r_1 s_3)^2$ is four times square of the triangle formed by vectors $\boldsymbol{r}$ and $\boldsymbol{s}$, we could replace it in equation (21) by $r^2 s^2 \sin^2\theta$, and obtain

$$V_{\mathrm{c}}(\boldsymbol{r}, \boldsymbol{s}) = \frac{\lambda^2}{2} \left(\frac{1}{r^2} + \frac{1}{s^2} \right) \frac{1}{\sin^2\theta}, \tag{22}$$

which is the same as the quantum mechanical centrifugal potential U if we set $\lambda = (D-3)/2$, see equation (V.17) from the review paper.

Minimization of T given by equation (20) in respect to momenta p_1, p_3, q_1, q_3 under a remaining constraint, equation (7), gives $p_1 = p_3 = q_1 = q_3 = 0$ and

$$T = V_{\mathrm{c}}(\boldsymbol{r}, \boldsymbol{s}). \tag{23}$$

Finally, we need to find minimum of the effective potential

$$V_{\mathrm{eff}}(\boldsymbol{r}, \boldsymbol{s}) = V_{\mathrm{c}}(\boldsymbol{r}, \boldsymbol{s}) + V(\boldsymbol{r}, \boldsymbol{s}), \tag{24}$$

in respect to coordinates, which is formally the same as the quantum energy in the limit of $D \to \infty$.

B. Properties of a matrix of tensor of four dimensional angular momentum under change of coordinate system

Here, we prove that in a certain coordinate system that does not change the form of a matrix given by equation (2), vectors of coordinates $\boldsymbol{r}$ and $\boldsymbol{s}$ will lie in $(1, 3)$ plane. This fact is used above in section II A to simplify equations for minimizing the energy.

For this purpose, we notice firstly that certain combinations of components of the matrix L are invariant under transformations of a coordinate system, for example an analogue of square of momentum,

$$\mathcal{L}^2 = \frac{1}{2} \sum_{i,j} L_{ij}^2. \tag{25}$$

Here, we introduce two another positive invariants

$$\mathcal{K}_{\pm} = \frac{1}{4} \sum_{i,j} \left(L_{ij} \pm \overline{L}_{ij} \right)^2, \tag{26}$$

where

$$\overline{L}_{ij} = \frac{1}{2} \sum_{k,l} \epsilon_{ijkl} L_{kl}, \tag{27}$$

and ϵ_{ijkl} is 1, -1 or 0 depending on parity of the permutation.

Since $\mathcal{K}_{-} = 0$ for the matrix given by equation (25), it will stay zero in any coordinate system. Since it is a sum of squares according to equation (26), each term separately is zero too, which means that $L_{ij} = \overline{L}_{ij}$ for any i, j, for example $L_{12} = L_{34}$, $L_{13} = L_{24}$ etc. Now, let us choose axes 1 and 3 of the coordinate system in the plane of the triangle formed by the nucleus and electrons, and axes 2 and 4 in the orthogonal complement to this plane. If we rotate the axes 2 and 4, then the components L_{12} and L_{14} will transform as coordinates of a two-dimensional vector, so that we can always make $L_{14} = 0$, and $\overline{L}_{14} = L_{23} = 0$ too. Note that both L_{13} and L_{24} are already zero because the axes 1 and 3 lie in the triangle plane. The remaining non-zero components L_{12} and $L_{34} = \overline{L}_{12}$ are equal. To find their value, it is convenient to use the fact that the invariant given by equation (25) is $\mathcal{L}^2 = 2\lambda^2$. It follows that in new coordinates, both L_{12} and L_{34} are either λ or $-\lambda$, i.e. the matrix is basically unchanged (since an overall sign is unimportant for minimization).

C. Non-existence of a one-electron motion with the angular momentum given by equation (2)

We prove here that just for one electron in four-dimension space, the tensor of angular momentum is never given by the matrix (2). If we choose axes 1 and 2 in the plane of vectors of coordinate and momentum of the electron, then L is given by the matrix

$$\mathsf{L} = \begin{pmatrix} 0 & l & 0 & 0 \\ -l & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{28}$$

where l is the angular momentum is this plane. Since the invariant given by equation (25), $\mathcal{K}_- = l^2 \neq 0$ for this case, it will stay non-zero in any coordinate system, so the matrix cannot be transformed into (2) for which $\mathcal{K}_- = 0$.