Bohr model for many-electron atoms in many dimensions[1]

Allowing dimensionality of space to be arbitrary large, we arrive to a highly symmetric electronic configuration, where each shell forms a regular multidimensional simplex. It allows us to minimize the configuration only over two parameters for each shell, radius of the simplex and its displacement in respect to the nucleus. For each shell, our configuration is reminiscent of a completely symmetric configuration considered by J. Loeser[2], but unlike Loeser's case, our total configuration is a superposition of several simplexes, one simplex for each shell.

I. BOHR MODEL FOR AN ATOM WITH N ELECTRONS

For a given number of electrons N and nuclear charge Z ($Z = N$ for a neutral atom), the functional of energy is defined as

$$W = W_1 + W_2, \tag{1}$$

where

$$W_1 = \sum_{i=1}^{N} \left(\frac{n_i^2}{2r_i^2} - \frac{Z}{r_i} \right), \tag{2}$$

$$W_2 = \sum_{i<j} \frac{1}{r_{ij}}, \tag{3}$$

$$r_i = |\boldsymbol{r}_i|, \quad r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|. \tag{4}$$

In (2), n_i for $i = 1, 2, 3, \ldots, N$ is a principal quantum number of i-th electron. The energy W is minimized in respect to vectors $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N$.

II. MANY-DIMENSIONAL BOHR MODEL

Bohr energies for large atoms could be lowered by minimizing in infinitely-dimensional space instead of three dimensional. The results for neon atom with 10 electrons are shown in Table II. With increasing of dimensionality, electronic shells became more and more symmetric, until finally at sufficiently large dimensionality they form a regular multidimensional simplex, with all distances between electrons of the same shell and the nucleus equal. For atoms with more than one electron in the outer shells, all simplexes appear to be co-centric

TABLE I. Dependence of energy and distances from electrons to the nucleus on dimensionality for argon atom (10 electrons). Numbers in paranthesis indicate multiplicity.

D	E	Distances for the first shell (two electrons)	Distances for the second shell (8 electrons)
1	−118.2194	0.1021(2)	0.4819(2), 0.9900(2), 2.1864(2), 6.2484(2)
2	−124.3432	0.102 471 78, 0.102 471 83	0.5801(2), 0.6120(2), 0.6365, 1.8967, 1.9517(2)
3	−126.0531	0.102 609, 0.102 625	0.6563(2), 0.6641(2), 0.6670, 0.6927, 0.7135, 3.7811
4	−126.8254	0.1027(2)	0.6845(6), 0.7931(2)
5	−127.0972	0.10271, 0.10274	0.6899(3), 0.7019(4), 0.7569
6	−127.3218	0.10273, 0.10274	0.6958(3), 0.6987(3), 0.7118(2)
7	−127.5343	0.1027(2)	0.6984(8)
≥ 8	−127.6237	0.1028(2)	0.6958(8)

with the nucleus and mutually orthogonal, and the energy function could be expressed through M radii if shells, where M is the number of shells. Since the dimensionality of each simplex equals to number of vertexes minus one, the total dimensionality equals to $Z - M$. For example, for neon atom,

$$W = -\frac{39}{2R_1} + \frac{7\sqrt{7}}{R_2} - \frac{80}{R_2} + \frac{1}{R_1^2} + \frac{16}{R_2^2} + \frac{16}{\sqrt{R_1^2 + R_2^2}},$$

and the total dimensionality is 8. The maximum number of minimization variables equals to the number of shells for the heaviest element, which is 7.

If the outer shell has only one electron, then it could be considered as zero-dimensional simplex. Since this electron should reside at certain distance from the nucleus, this simplex is shifted in a certain direction. In this case, as a result of electronic interaction, other simplexes corresponding to inner shells are no longer co-centric. It appears that they are shifted in the same direction which is orthogonal to all simplexes. Any inner shell is characterized by two parameters, (R, d), where R is the radius of the simplex, and d is the shift, with distances between electrons and the nucleus equal to $\sqrt{R^2 + d^2}$. The outer shell is characterized by just one parameter, the shift d. Thus, for atom with M shells there are in total $2M - 1$ parameters of minimization, and the total dimensionality is $Z - M + 1$. For example, for

sodium atom, the energy function is expressed through 5 variables, R_1, R_2, d_1, d_2, d_3:

$$W = \frac{2}{\sqrt{(d_1-d_3)^2+R_1^2}} - \frac{88}{\sqrt{d_2^2+R_2^2}} + \frac{8}{\sqrt{(d_2-d_3)^2+R_2^2}} + \frac{16}{\sqrt{(d_1-d_2)^2+R_1^2+R_2^2}} - \frac{11}{d_3} + \frac{1}{2R_1} + \frac{7\sqrt{7}}{R_2} + \frac{16}{d_2^2+R_2^2} + \frac{9}{2d_3^2} - \frac{22}{\sqrt{d_1^2+R_1^2}} + \frac{1}{d_1^2+R_1^2},$$

and the total dimensionality is 9.

In the model considered by Loeser[2], all electrons are equivalent. The kinetic energy term is different from our model. Particularly, it turns to infinity if the electrons and the nucleus form a polytope of dimensionality less than Z. It appears that electrons form a regular $Z-1$-dimensional simplex, and the nucleus is shifted in direction of Z-th dimension in respect to the center of the simplex. In this case, the electronic configuration is described only by two parameters, R and d, or alternatively by R and θ as in [2].

Errors of Bohr model in three dimensions and in many dimensions are shown on Fig. 1, juxtaposed on the plot taken from the paper[2]. Bohr model in many dimensions lowers the energy in comparison with $3D$-model, and it gives better accuracy 1.5% for large Z, instead of 4.3% for $3D$-model. Unlike Loeser's model, our approximation over-estimates energy for small Z and under-estimates it for large z. Since our approximation is just zero-order classical limit, it does not exhibit unphysical fine structure which arises from changing vibrational state[2].

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[1] The most recent version of these notes is available through Internet at address http://www.asergeev.com/files/tamu/larged.pdf.

[2] J.G. Loeser. J. Chem. Phys. **86**, 5635 (1987).

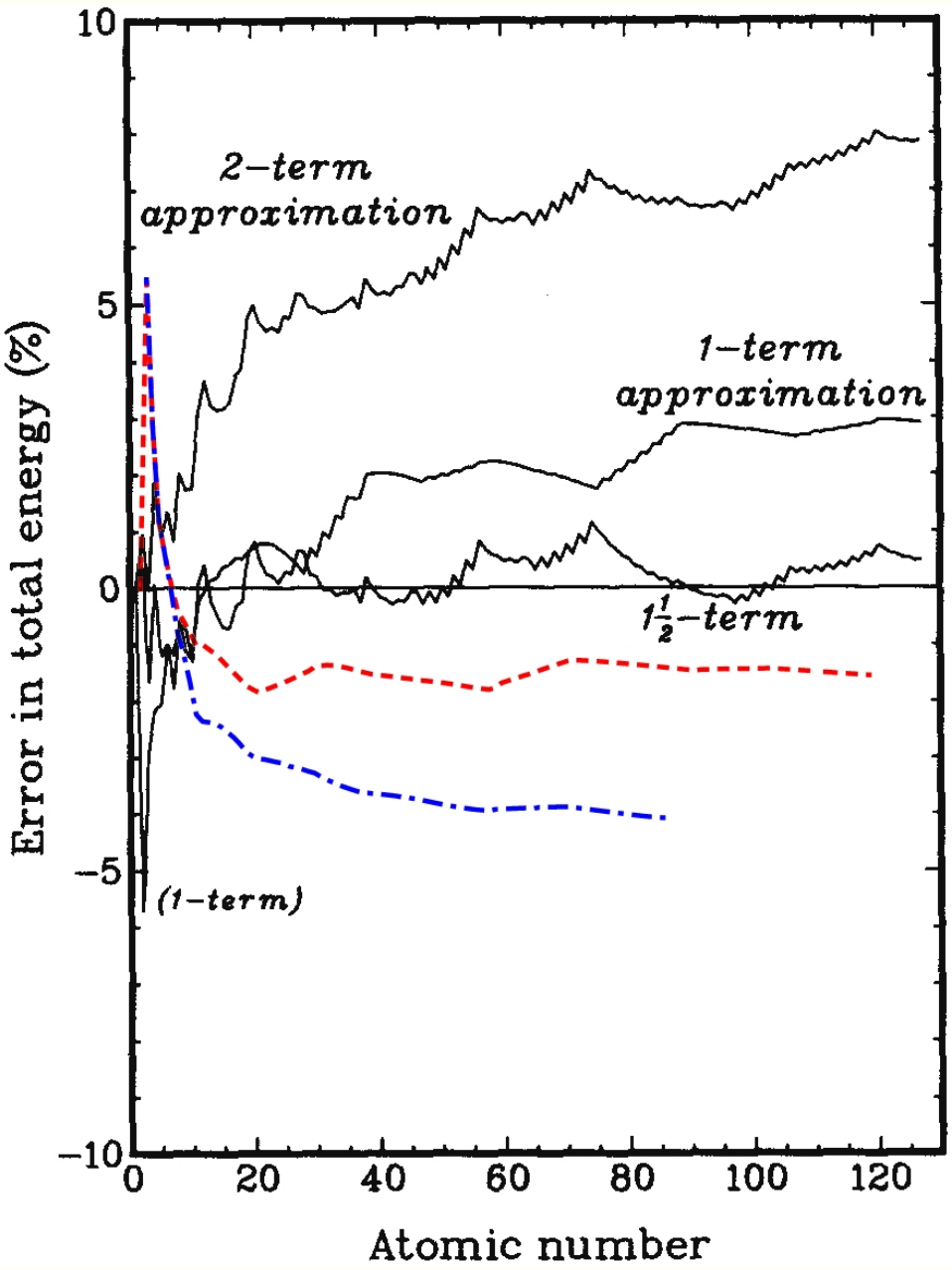

FIG. 1. Accuracy of Bohr model as a function of Z. Solid lines are approximations introduced in [2]. Dot-dashed line are results of the Bohr model based on a minimization of classical configurations in three dimensional space, and dashed line in multidimensional space.