Mathematical Analysis of a Bohr Atom Model

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Abstract

N. Bohr proposed in 1913 a model for atoms and molecules by synthesizing Planck's quantum hypothesis with classical mechanics. When the atom number Z is small, his model provides good accuracy for the ground state energy. When Z is large, his model is not as accurate but still provides a good trend agreeing with the experimental values of the ground state energy of atoms.

The main objective of this paper is to provide a rigorous mathematical analysis for the Bohr atom model. We have established the following:

(1) An existence proof of the global minimizer of the ground state energy through scaling;

(2) A careful study of the critical points of the energy function. Such critical points include both the stable steady-state electron configurations as well as unstable saddle-type configurations.

(3) Coplanarity of certain electron configurations.

Numerical examples and graphics are also illustrated.

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1 Introduction

In 1913, N. Bohr published a series of three papers [1, 2, 3] describing his approach for modeling atoms and molecules by synthesizing Planck's quantum hypothesis with classical mechanics. Bohr tried to explain the hydrogen spectral lines with a radical "planetary" model of electrons orbiting around a nucleus. He made a set of assumptions to quantify his model, leading to the existence in the atom a discrete set of stable, stationary orbits for electrons:

(1) The dynamical equilibrium of the stationary orbits is achieved by balancing the electrostatic Coulomb forces of attraction against the centrifugal effect and the interelectronic repelling of the orbital motion in classical mechanics.

(2) Stationary states satisfy the quantization condition that the ratio of the total kinetic energy of the electron to its orbital frequency be an integral multiple of $\pi\hbar$. For circular orbits, this signifies that the angular momentum of the electron is restricted to integral multiples of $\hbar$.

(3) Energy is emitted only when an electron makes a "jump" (i.e., non-continuous) transition between two stationary orbits, and the frequency of such a radiation emission is determined by $\Delta E/2\pi\hbar$, where ΔE is the energy difference between the two orbits where the transition occurs.

From now on, vectors will be denoted by bold letters. For the hydrogen atom, Bohr's assumptions work as follows. The total energy of the electron on a circular orbit with radius r and velocity $\boldsymbol{v}$ is

$$\begin{aligned} E &= \text{kinetic energy} + \text{potential energy} \\ &= \frac{m_e v^2}{2} - \frac{Ze^2}{r}, \end{aligned} \tag{1.1}$$

where

$$\begin{aligned} m_e &= \text{the mass of the electron,} \\ e &= \text{the charge of the electron,} \\ Ze &= \text{the positive charge of the nucleus.} \end{aligned}$$

Since

$$\begin{aligned} \boldsymbol{L} &= \text{the angular momentum} \\ &= \boldsymbol{r} \times \boldsymbol{p} \qquad (\boldsymbol{p} \equiv \text{the linear momentum} = m_e\boldsymbol{v}), \\ |\boldsymbol{L}| &= L = m_e v r, \end{aligned} \tag{1.2}$$

which, in turn, by Bohr's quantization assumption, satisfies

$$L = n\hbar. \tag{1.3}$$

From (1.1)–(1.3), we now have

$$\begin{aligned} E &= \frac{m_e^2 v^2 r^2}{2m_e r^2} - \frac{Ze^2}{r} \\ &= \frac{L^2}{2m_e r^2} - \frac{Ze^2}{r} \\ &= \frac{n^2\hbar^2}{2m_e r^2} - \frac{Ze^2}{r} \\ &= \frac{1}{2}\frac{n^2}{r^2} - \frac{Z}{r}, \end{aligned} \tag{1.4}$$

in atomic units (by setting $e = 1, \hbar^2/m_e = 1$).

Electron numbers i	Electron shells names	Assigned quantum numbers n_i
$1 \le i \le 2$	K	1
$3 \le i \le 8$	L	2
$9 \le i \le 18$	M	3
$19 \le i \le 36$	N	4
$37 \le i \le 54$	O	5
$55 \le i \le 86$	P	6
$87 \le i \le 108$	Q	7

(1.5)

Table 1. Assignment of quantum numbers n_i for the ground state of an atom with atom number Z from $Z = 1$ to 108.

Minimizing $E = E(r, n, Z)$ with respect to r for $n = 1, 2, 3, \ldots$, for fixed Z, we obtain

$$\widehat{E}_n \equiv \min_{r>0} E(r, n, Z) = -\frac{1}{2}\frac{Z^2}{n^2}, \qquad n = 1, 2, 3, \ldots \ . \tag{1.6}$$

These values and their differences totally determine the hydrogen atom's spectral lines.

Sommerfeld later in 1916 generalized Bohr's theory by allowing non-circular orbits and by incorporating relativistic effects, leading to the Bohr–Sommerfeld (old) quantum theory of the hydrogen atom. However, for other atoms, including the simple helium, there are difficulties unaccountable by the Bohr–Sommerfeld theory; see e.g. [6, 7]. Heisenberg worked under both Bohr and Sommerfeld trying to resolve such difficulties, eventually gave up but in the process invented the matrix mechanics during the 1930s.

The objective of the present paper is to analyze, mathematically, a Bohr atom model for the ground-states of general atoms. Such a general Bohr model seems to be well understood by atomic physicists (see, e.g., the pictorials on the website of Patton [11]) but we could not provide an exact citation. The model that we are going to describe below is communicated to us by our colleague, Dr. S.A. Chin [4]. Consider a neutral atom with atom number Z. There are Z electrons. The kinetic energy of an electron i moving around a circular orbit of radius r_i on the n-th shell, $n_i = 1, 2, 3, \ldots$, is

$$T_i = -\frac{1}{2}n_i^2/r_i^2, \qquad (r_i = |\boldsymbol{r}_i|, \boldsymbol{r}_i = (x_i, y_i, z_i) \in \mathbb{R}^3 \text{ is the position vector of electron } i) \tag{1.7}$$

For a heuristic derivation of (1.7), see [6, Appendix]. The potential energy is attributed to the Coulomb interactions of electron j with the nucleus and electrons j for $j \neq i$:

$$P_i = -\frac{Z}{r_i} + \sum_{\substack{j=1 \\ j\neq i}}^{Z} \frac{1}{r_{ij}} \qquad (r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|). \tag{1.8}$$

Thus the total energy of the atom is

$$\begin{aligned} E = E(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_Z) &= \sum_{j=1}^{Z}(T_j + P_j) \\ &= \sum_{i=1}^{Z}\left(\frac{n_i^2}{2r_i^2} - \frac{Z}{r_i}\right) + \sum_{\substack{i,j=1 \\ i\neq j}}^{Z} \frac{1}{2r_{ij}}. \end{aligned} \tag{1.9}$$

We now pack these Z electrons into the various "electron shells" by the *Aufbau Principle*[1] by assigning the values of n_i according to Table 1. These designated integral values of n_i give us the Bohr atom model in this paper.

The stable stationary orbit or electron configuration, denoted as $(\boldsymbol{r}_1^*, \boldsymbol{r}_2^*, \ldots, \boldsymbol{r}_Z^*)$, and the associated ground state energy $E(\boldsymbol{r}_1^*, \boldsymbol{r}_2^*, \ldots, \boldsymbol{r}_Z^*)$, can now be obtained by

$$\min_{\boldsymbol{R}\in\mathbb{R}^{3Z}} E(\boldsymbol{R}) \equiv E(\boldsymbol{R}^*), \quad \boldsymbol{R}^* \equiv (\boldsymbol{r}_1^*, \boldsymbol{r}_2^*, \ldots, \boldsymbol{r}_Z^*). \tag{1.10}$$

In Table 2, we have listed the ground-state energy of all the atoms calculated from (1.10) as well as the known ("exact") experimental values. The reader may find some agreement between these two sets of values, especially when Z is small.

The Bohr model of atoms was derived by Bohr in an *ad hoc* way at first. The rigorous, wave-mechanical model is the following Schrödinger–Born–Oppenheimer equation describing the many-particle quantum-mechanical behavior

$$\left(-\frac{1}{2}\sum_{k=1}^{Z} \nabla_k^2 + \frac{1}{2}\sum_{\substack{k,k'=1 \\ k\neq k'}}^{Z} \frac{1}{r_{kk'}} - \sum_{k=1}^{Z} \frac{Z}{r_k} \right) \phi(\boldsymbol{R}) = E\phi(\boldsymbol{R}). \tag{1.11}$$

As Bohr's model appears to be something of the history, why does it still warrant any attention? The reasons that motivate our study here are three fold:

(i) Recently, through the *dimensional scaling* (D-scaling) method [8], Svidzinsky, Scully and Herschbach [12, 13] have arrived at Bohr's model from the totally quantum-mechanical (Schrödinger–Born–Oppenheimer) model via asymptotics. This has stirred surprise, excitement and interests [15], especially among the researchers in the Institute for Quantum Studies at Texas A&M and has rekindled efforts in trying to understand the synergism between D-scaling, the Schrödinger–Born–Oppenheimer model and the Bohr model for atoms and molecules.

(ii) The Schrödinger–Born–Oppenheimer model (1.11) involves large-scale numerical computation and is rather theoretically intractable, while the Bohr model (1.5), (1.9) and (1.10) requires only desk-top computing, producing outcomes of electron configurations highly valuable and intuitive for atomic experiments and molecular modeling, especially with the incorporation of the Hartree–Fock and other refinement techniques ([6, 7, 5, 10, 14], e.g.).

(iii) Mathematically speaking, even though Bohr's atom model is nearly 90 years old, historically it has not attracted due attention in the mathematics community and, thus, has not undergone rigorous mathematical analysis it rightfully deserves. Many interesting mathematical problems are worth investigation. We hope our mathematical analysis carried out here will improve the understanding of Bohr's atomic model and that of atoms in general at a more fundamental level, with an ultimate goal of improving the modeling and compution of molecules or even building new molecular models.

2 Existence and Algorithm for the Global Minimizer

The following problems are of significant mathematical interests, which also have physical importance:

[1]The packing of electrons into electron shells by the Aufbau Principle involves also *subshells* $p.d.f$, etc. Since here we are only dealing with ground states of atoms, we pack electrons only into the *principal* s shells.

(i) A rigorous existence proof of ground state energies;

(ii) *Stable* as well as *unstable* electron steady-state orbits;

(iii) Geometric configurations: co-planarity and symmetries of electron locations.

We discuss them through a sequence of lemmas and theorems.

From now on, to simplify notation, we often write

$$\sum_{i=1}^{n} \text{ as } \sum_{i}, \quad \sum_{\substack{i,j=1 \\ i\neq j}}^{n} \text{ as } \sum_{i\neq j},$$

unless more clarity of the summation index is deemed necessary.

We begin by letting Z be a positive number and n be a positive integer; $n = 1, 2, 3, \ldots$, define

(1) For $n = 1$,

$$E_1^Z\colon\ \mathbb{R}^3 \to \mathbb{R}, \quad E_1^Z(\boldsymbol{r}_1) = \frac{n_1^2}{2r_1^2} - \frac{Z}{r_1}, \qquad \boldsymbol{r}_1 \in \mathbb{R}^3;$$

(2) For $n \geq 2$ and $Z \geq n$, $E_n^Z : \mathbb{R}^{3n} \to \mathbb{R}$,

$$E_n^Z(\mathbf{R}) = \sum_{i=1}^{n} \left(\frac{n_i^2}{2r_i^2} - \frac{Z}{r_i} \right) + \sum_{\substack{i,j=1 \\ i\neq j}}^{n} \frac{1}{2r_{ij}}, \tag{2.1}$$

where $\boldsymbol{R} = (\boldsymbol{r}_1, ..., \boldsymbol{r}_n)$, $\boldsymbol{r}_i \in \mathbb{R}^3$, r_i and r_{ij} are defined as in (1.7) and (1.8). The domain of E_n^Z is then given by $\mathbb{R}^{3n}\backslash\mathcal{S}_n$, where $\mathcal{S}_n$ is the singularity manifold of E_n^Z given by

$$\mathcal{S}_n = \{\boldsymbol{R} = (\boldsymbol{r}_1, ..., \boldsymbol{r}_n) \in \mathbb{R}^{3n} \;\Big|\; \boldsymbol{r}_j = \mathbf{0} \text{ or } \boldsymbol{r}_j - \boldsymbol{r}_k = 0, \text{ for some } j, k, 1 \leq j, k \leq n, j \neq k\}.$$

E_n^Z is obviously in $C^\infty(\mathbb{R}^{3n}\backslash\mathcal{S}_n)$. We are interested in the existence of $\boldsymbol{R}^* \in \mathbb{R}^{3n}\backslash\mathcal{S}_n$ such that

$$E_n^Z(\boldsymbol{R}^*) = \inf_{\boldsymbol{R}\in\mathbb{R}^{3n}\backslash\mathcal{S}_n} E_n^Z(\boldsymbol{R}), \quad \text{for} \quad n \geq 2.$$

Note that the case of $n = 1$ is already solved in (1.6). From now on, we will abbreviate E_n^Z as E if no ambiguities should arise. Throughout the rest of the section, the reader may find that in all of the proofs given, as long as $n_i > 0$ for $i = 1, 2, \ldots, n$, then the proofs go through without any problem, i.e., n_i's do not have to follow the designated values as in Table 1. We further define

$$\mathcal{S}_Z^n = \left\{ \boldsymbol{R} \in \mathbb{R}^{3n}\backslash\mathcal{S}_n \;\Big|\; \sum_i \frac{Z}{r_i} - \sum_{i\neq j} \frac{1}{2r_{ij}} > 0 \right\}.$$

Lemma 1 (Scaling along a ray). *Let $\boldsymbol{R} \in \mathcal{S}_Z^n$. The function $g\colon\ \mathbb{R}_+ \equiv (0, \infty) \to \mathbb{R}$, $g(t) \equiv E(t\boldsymbol{R})$ has a unique global minimum at*

$$t^* = t^*(\boldsymbol{R}) = arg \min_{t\neq 0, t\in\mathbb{R}} E(t\boldsymbol{R}), \tag{2.2}$$

where

$$t^* > 0, g'(t^*) = 0, \quad g''(t^*) > 0, \tag{2.3}$$

$$E(t^*\boldsymbol{R}) = -\frac{1}{2}\sum_i \frac{n_i^2}{r_i^2}\frac{1}{t^{*2}} = -\frac{1}{2}\left(\sum_i \frac{Z}{r_i} - \sum_{i\neq j} \frac{1}{r_{ij}} \right)^2 \Big/ \left(\sum_i \frac{n_i^2}{r_i^2} \right) < 0. \tag{2.4}$$

Proof. First, we note that $\mathcal{S}_Z^n$ is a nonempty unbounded open set of $\mathbb{R}^{3Z}$. It is easy to see that if $\boldsymbol{R} \in \mathcal{S}_Z^n$, then $t\boldsymbol{R} \in \mathcal{S}_Z^n$ for any $t \neq 0$, i.e., $\mathcal{S}_Z^n$ is star-shaped. For $t > 0$, we have

$$g(t) = \frac{1}{t^2} \sum_i \left(\frac{n_i^2}{2r_i^2} \right) + \frac{1}{t} \left(-\sum_i \frac{Z}{r_i} + \sum_{i \neq j} \frac{1}{2r_{ij}} \right), \tag{2.5}$$

$$g'(t) = -\frac{2}{t^3} \sum_i \frac{n_i^2}{2r_i^2} + \frac{1}{t^2} \left(\sum_i \frac{Z}{r_i} - \sum_{i \neq j} \frac{1}{2r_{ij}} \right). \tag{2.6}$$

Set $g'(t^*) = 0$ to get the *only* zero of g' at

$$t^* = \frac{\sum_i \frac{n_i^2}{r_i^2}}{\sum_i \frac{Z}{r_i} - \sum_{i \neq j} \frac{1}{2r_{ij}}}. \tag{2.7}$$

Note that the denominator in (2.7) is positive since $\boldsymbol{R} \in \mathcal{S}_Z^n$. So t^* is well-defined. Next, we have

$$g''(t) = \frac{6}{t^4} \sum_i \frac{n_i^2}{2r_i^2} - \frac{2}{t^3} \left(\sum_i \frac{Z}{r_i} - \sum_{i \neq j} \frac{1}{2r_{ij}} \right),$$

$$g''(t^*) = \frac{1}{t^{*4}} \sum_i \frac{n_i^2}{r_i^2} > 0.$$

Therefore $g(t)$ has only a global minimum at $t^* > 0$, and $\phi(t^*) = E(t^*\boldsymbol{R})$ is given as in (2.4). □

Remark 1. If $\boldsymbol{R} \notin \mathcal{S}_n \cup \mathcal{S}_Z^n$, then for $t > 0$,

$$g(t) = E(t\boldsymbol{R}) = \frac{1}{t^2} \sum_i \frac{n_i^2}{r_i^2} + \frac{1}{t} \left(-\sum_i \frac{Z}{r_i} + \sum_{i \neq j} \frac{1}{2r_{ij}} \right).$$

This function $g(t)$ is always *positive* and monotonic for $t \in (0, \infty)$ such that $g'(t) = 0$ has no solution $t \in \mathbb{R}_+$. In fact, $g'(t) < 0$ on $\mathbb{R}_+$, i.e., g is strictly decreasing. Since $g(t)$ is smooth on $\mathbb{R}_+$, $\lim_{t \to 0} g(t) = +\infty$ and $\lim_{t \to \infty} g(t) = 0$, we have $g(t) \geq 0$ for any $t \in \mathbb{R}_+$. □

From (2.1), by completing the square we have

$$E(\boldsymbol{R}) = \sum_i \left(\frac{n_i}{\sqrt{2}\, r_i} - \frac{\sqrt{2}\, Z}{n_i} \right)^2 + \sum_{i \neq j} \frac{1}{2r_{ij}} - \sum_i \frac{2Z^2}{n_i^2} \geq -\sum_i \frac{2Z^2}{n_i^2},$$

therefore $E(\boldsymbol{R})$ is bounded from below, its infimum exists and we have

$$\mu_n^Z := \inf_{\boldsymbol{R} \in \mathbb{R}^{3n} \setminus \mathcal{S}_n} E_n^Z(\boldsymbol{R}) = \inf_{\boldsymbol{R} \in \mathcal{S}_Z^n} E_n^Z(\boldsymbol{R}) < 0. \tag{2.8}$$

We introduce the following gradient notation: Let $f(x_1, x_2, \ldots, x_n)$ be any scalar valued function of n variables. For any variables $x_{i_1} x_{i_2}, \ldots, x_{i_k}$, where $1 \leq i_1 < i_2 < \cdots < i_k \leq n$, we denote the

gradient of f with respect to these variables as

$$D_{(x_{i_1}x_{i_2},\ldots,x_{i_k})}f(x_1,x_2,\ldots,x_n)=\begin{bmatrix}\dfrac{\partial f}{\partial x_{i_1}}(x_1,x_2,\ldots,x_n)\\ \dfrac{\partial f}{\partial x_{i_2}}(x_1,x_2,\ldots,x_n)\\ \vdots\\ \dfrac{\partial f}{\partial x_{i_k}}(x_1,x_2,\ldots,x_n)\end{bmatrix},$$

which is regarded as a column vector. If $(x_{i_1},x_{i_2},\ldots,x_{i_k})=(x_1,x_2,\ldots,x_n)$, i.e., all the variables $x_1,x_2,\ldots,x_n$ are included, then we simply write the above as Df, i.e.,

$$Df=[\partial f/\partial x_1 \quad \partial f/\partial x_2\ldots\partial f/\partial x_n]^T$$

(where T means transpose). A point $\boldsymbol{y}\in\mathbb{R}^n$ is said to be a *critical point* of f if $Df(y)=\mathbf{0}$. Obviously, any local or global maximum or minimum of E is a critical point, but many critical points of E may be of the saddle type which are *physically unstable*.

Later, we will also need to utilize the *Hessian matrix* of f. The Hessian matrix H of f is an $n\times n$ matrix whose (i,j)-entry, H_{ij}, is $H_{ij}\equiv\partial^2 f/(\partial x_i\partial x_j)$. We denote the Hessian as D^2f, i.e.,

$$D^2f=\left[\frac{\partial^2 f}{\partial x_i\partial x_j}\right]_{1\le i,j\le n}. \tag{2.9}$$

A critical point $\boldsymbol{R}^\dagger\in\mathbb{R}^{3Z}$ of $E(\boldsymbol{R})$ is defined by $DE(\boldsymbol{R}^\dagger)=\mathbf{0}$. Thus, at a critical point we obtain the set of gradient (vector) equations

$$D_{\boldsymbol{r}_j}E(\boldsymbol{R}^\dagger)=\mathbf{0}\quad\text{for}\quad j=1,2,\ldots,n, \tag{2.10}$$

i.e.,

$$\left(\frac{n_j^2}{r_j^{\dagger 4}}-\frac{Z}{r_j^{\dagger 3}}\right)\boldsymbol{r}_j^\dagger+\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{2r_{kj}^{\dagger 3}}\boldsymbol{r}_{kj}^\dagger=\mathbf{0}\in\mathbf{R}^3,\qquad j=1,2,\ldots,n. \tag{2.11}$$

Using $\boldsymbol{r}_{kj}^\dagger=\boldsymbol{r}_k^\dagger-\boldsymbol{r}_j^\dagger$, we can write (2.11) alternatively as

$$\left(\frac{n_j^2}{r_j^{\dagger 4}}-\frac{Z}{r_j^{\dagger 3}}+\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{2r_{kj}^{\dagger 3}}\right)\boldsymbol{r}_j^\dagger-\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{2r_{kj}^{\dagger 3}}\boldsymbol{r}_k^\dagger=\mathbf{0},\qquad j=1,2,\ldots,n. \tag{2.12}$$

These constitute the equations for the *steady states* of electron orbits, based on the Bohr model. In particular, if $\boldsymbol{R}^*$ is a global minimum of E established in the preceding section, then $\boldsymbol{R}^*$ is necessarily a critical point and so the equations in (2.11) or (2.12) hold, with the "†" signs therein replaced by "$*$"s.

Theorem 1 (Virial). *Let $\boldsymbol{R}^\dagger=(\boldsymbol{r}_1^\dagger,\boldsymbol{r}_2^\dagger,\ldots,\boldsymbol{r}_n^\dagger)$ be a critical point of E satisfying $DE(\boldsymbol{R}^\dagger)=\mathbf{0}\in\mathbb{R}^{3n}$, then so is $\mathcal{R}\boldsymbol{R}^\dagger$ for any 3-D rotation $\mathcal{R}$, and $\boldsymbol{R}^\dagger\in\mathcal{S}_Z^n$. The ground state energy value is given by*

$$E(\boldsymbol{R}^\dagger)=-\sum_{i=1}^{n}\frac{n_i^2}{2r_i^{\dagger 2}}<0. \tag{2.13}$$

In addition, along the ray $t\boldsymbol{R}^\dagger$ for $t>0$, $E(t\boldsymbol{R}^\dagger)$ attains its global minimum at $t=1$.

Proof. Consider, for $t \neq 0$,

$$E(t\boldsymbol{R}^\dagger) = \sum_{i=1}^{n} \left(\frac{n_i^2}{2t^2 r_i^{\dagger 2}} - \frac{Z}{t r_i^\dagger} \right) + \sum_{\substack{i,j=1 \\ i \neq j}}^{2} \frac{1}{2t r_{ij}^\dagger}.$$

Then, because $DE(\boldsymbol{R}^\dagger) = \mathbf{0}$, we have

$$\frac{d}{dt} E(t\boldsymbol{R}^\dagger)\big|_{t=1} = DE(\boldsymbol{R}^\dagger) \cdot \boldsymbol{R}^\dagger = 0,$$

i.e.,

$$\sum_i \left(-\frac{n_i^2}{r_i^{\dagger 2}} + \frac{Z}{r_i^\dagger} \right) - \sum_{i \neq j} \frac{1}{2r_{ij}^\dagger} = 0, \tag{2.14}$$

and

$$\sum_i \frac{Z}{r_i^\dagger} - \sum_{i \neq j} \frac{1}{2r_{ij}^\dagger} = \sum_i \frac{n_i^2}{r_i^{\dagger 2}} > 0,$$

and, hence, $\boldsymbol{R}^\dagger \in \mathcal{S}_Z^n$. Therefore

$$\begin{aligned} E(\boldsymbol{R}^\dagger) &= \sum_i \left(\frac{n_i^2}{2r_i^{\dagger 2}} - \frac{Z}{r_i^\dagger} \right) + \sum_{i \neq j} \frac{1}{2r_{ij}^\dagger} \\ &= \left[\sum_i \left(\frac{n_i^2}{r_i^{\dagger 2}} - \frac{Z}{r_i^\dagger} \right) + \sum_{i \neq j} \frac{1}{2r_{ij}} \right] - \sum_i \frac{n_i^2}{2r_i^{\dagger 2}} \\ &= -\sum_{i=1}^{Z} \frac{n_i^2}{2r_i^{\dagger 2}}. \end{aligned}$$

But from the proof of Lemma 1, the derivative of function $g(t) = E(t\boldsymbol{R}^\dagger)$, $g'(t)$, has only one zero t^* satisfying $g'(t^*) = 0$. Thus $t^* = 1$, and $t^* = 1$ necessarily corresponds to the global minimum of $g(t)$.

The proof is complete. □

Corollary 1. *Let $\boldsymbol{R}^\dagger = (\boldsymbol{r}_1^\dagger, \ldots, \boldsymbol{r}_n^\dagger)$ be a critical point of E satisfying Theorem 1. Define an $n \times n$ matrix $M^\dagger$ whose (j,k)-entries M_{jk} are given by*

$$M_{jk}^\dagger = \begin{cases} -\dfrac{1}{2r_{kj}^{\dagger 3}}, & k \neq j; \\ \dfrac{n_k^2}{r_k^{\dagger 4}} - \dfrac{Z}{r_k^{\dagger 3}} + \displaystyle\sum_{\substack{i=1 \\ i \neq k}}^{Z} \frac{1}{2r_{ki}^{\dagger 3}}, & j = k. \end{cases} \tag{2.15}$$

Then $\det M^\dagger = 0$.

Proof. Note that these $M_{jk}^\dagger$'s are the coefficients appearing in (2.12). As the matrix equation $M^\dagger \boldsymbol{\alpha} = \mathbf{0} \in \mathbb{R}^n$ has at least a nontrivial solution $\boldsymbol{\alpha} \in \mathbb{R}^n$, $\boldsymbol{\alpha} \neq \mathbf{0}$, where $\boldsymbol{\alpha}$ is a vector formed by all of the i^{th} components of the vectors in $(\boldsymbol{r}_1^\dagger, \boldsymbol{r}_2^\dagger, \ldots, \boldsymbol{r}_n^\dagger)$, with $i = 1$, or 2, or 3, we must have the determinant of $M^\dagger$ equal to 0. □

From (2.14), we obtain that the set

$$\mathcal{N}_Z^n = \left\{ \boldsymbol{R} = (\boldsymbol{r}_1, ..., \boldsymbol{r}_n) \in \mathbb{R}^{3n} \backslash \mathcal{S}_n \;\middle|\; \sum_{k=1}^{n} \left[\frac{Z}{r_k} - \frac{n_i^2}{r_k^2} \right] = \sum_{\substack{j,k=1 \\ j \neq k}}^{n} \frac{1}{2r_{jk}} \right\}, \tag{2.16}$$

contains all critical points of E_n^Z. $\mathcal{N}_Z^n$ is a closed nonempty subset of $\mathbb{R}^{3n}$, and $\mathcal{N}_Z^n \subset \mathcal{S}_Z^n$. We then have

$$\inf_{\boldsymbol{R} \in \mathcal{S}_Z^n} E_n^Z(\boldsymbol{R}) = \inf_{\boldsymbol{R} \in \mathcal{N}_Z^n} E_n^Z(\boldsymbol{R}). \tag{2.17}$$

Furthermore, we obtain from (2.4)

$$E_n^Z(\boldsymbol{R}) = -\frac{1}{2} \sum_{i=1}^{n} \frac{n_i^2}{r_i^2} < 0, \quad \forall \boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) \in \mathcal{N}_Z^n. \tag{2.18}$$

When $n = 1$, define $\mathcal{N}_Z^1 = \{ \boldsymbol{r}_1 \in \mathbb{R}^3 \;\big|\; r_1 = n_1^2/Z \}$. For any $\boldsymbol{r} \in \mathcal{N}_Z^1$,

$$E_1^Z(\boldsymbol{r}) = -\frac{Z^2}{2n_1^2} = \inf_{\boldsymbol{r}_1 \in \mathbb{R}^3 \backslash \mathcal{S}_1} E_1^Z(\boldsymbol{r}_1).$$

Lemma 2. *Let $n \geq 2$ and $Z = n$, then*

$$\mu_n^Z \leq \mu_k^Z, \quad \forall k\colon\ 1 \leq k \leq n-1.$$

If $\mu_k^Z = E_k^Z(\boldsymbol{r}_1^*, \ldots, \boldsymbol{r}_k^*)$ for some $(\boldsymbol{r}_1^*, \ldots, \boldsymbol{r}_k^*) \in (\mathbb{R}^3)^k$, then

$$\mu_n^Z < \mu_k^Z, \quad \forall 1 \leq k \leq n-1.$$

Proof. For any $(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k) \in \mathcal{S}_Z^k$ and $(\boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_n) \in \mathcal{S}_{Z-k}^{n-k}$, we have

$$\begin{aligned}
& E_n^Z(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k, t\boldsymbol{r}_{k+1}, \ldots, t\boldsymbol{r}_n) \\
= & \left\{ \sum_{j=1}^{k} \left[\frac{n_j^2}{2r_j^2} - \frac{Z}{r_j} \right] + \sum_{\substack{j,i=1 \\ j \neq i}}^{k} \frac{1}{2r_{ij}} \right\} \\
& + \left\{ \sum_{j=k+1}^{n} \left[\frac{n_j^2}{2t^2 r_j^2} - \frac{Z}{t r_j} \right] + \sum_{\substack{j,i=k+1 \\ j \neq i}}^{n} \frac{1}{2tr_{ij}} + \sum_{j=k+1}^{n} \sum_{i=1}^{k} \frac{1}{|t\boldsymbol{r}_j - \boldsymbol{r}_i|} \right\} \\
\equiv & \ \Delta_1 + \frac{1}{t} \Delta_2
\end{aligned}$$

Note that

$$\begin{aligned}
\lim_{t \to \infty} \Delta_2 &= \lim_{t \to \infty} \left\{ \sum_{j=k+1}^{n} \left[\frac{n_j^2}{2tr_j^2} - \frac{Z}{r_j} \right] + \sum_{\substack{j,i=k+1 \\ j \neq i}}^{n} \frac{1}{2r_{ij}} + \sum_{j=k+1}^{n} \sum_{i=1}^{k} \frac{t}{|t\boldsymbol{r}_j - \boldsymbol{r}_i|} \right\} \\
&= -\left(\sum_{j=k+1}^{n} \frac{Z-k}{r_j} - \sum_{\substack{j,i=k+1 \\ j \neq i}}^{n} \frac{1}{2r_{ij}} \right).
\end{aligned}$$

In the special case when $k = n-1$, we have $\boldsymbol{r}_n \in \mathcal{S}^1_{Z-n+1}$ and then

$$\lim_{t\to\infty} \Delta_2 = -\frac{Z-n+1}{r_n} < 0;$$

but if $1 \le k \le n-2$, which occurs only when $n \ge 3$, then $(\boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_n) \in \mathcal{S}^{n-k}_{Z-k}$ implies

$$\lim_{t\to\infty} \Delta_2 = -\left(\sum_{j=k+1}^{n} \frac{Z-k}{r_j} - \sum_{\substack{j,i=k+1 \\ j\neq i}}^{n} \frac{1}{2r_{ij}} \right) < 0. \tag{2.19}$$

Thus we obtain, for any $(\boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_n) \in \mathcal{S}^{n-k}_{Z-k}$

$$\frac{1}{t}\Delta_2 < 0, \quad \text{for } t \text{ sufficiently large.}$$

Hence, we have for any $(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k) \in \mathcal{S}^k_Z$, for t sufficiently large,

$$\mu^Z_n \le E^Z_n(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k, t\boldsymbol{r}_{k+1}, \ldots, t\boldsymbol{r}_n) < \left(\sum_{j=1}^{k} \left[\frac{n_j^2}{2r_j^2} - \frac{Z}{r_j} \right] + \sum_{\substack{j,i=1 \\ j\neq i}}^{k} \frac{1}{2r_{ij}} \right). \tag{2.20}$$

Thus

$$\mu^Z_n \le \mu^Z_k.$$

If $\mu^Z_k = E^Z_k(\boldsymbol{r}^*_1, \ldots, \boldsymbol{r}^*_k)$ for some $(\boldsymbol{r}^*_1, \ldots, \boldsymbol{r}^*_k) \in (\mathbb{R}^3)^k$, then (2.19) and (2.20) leads to

$$\mu^Z_n < \mu^Z_k.$$

□

Theorem 2. *Let $Z = n$. There exists an $\boldsymbol{R}^* = (\boldsymbol{r}^*_1, \ldots, \boldsymbol{r}^*_n) \in \mathbb{R}^{3n}$ such that*

$$E^Z_n(\boldsymbol{R}^*) = \inf_{\boldsymbol{R}\in\mathbb{R}^{3n}\setminus\mathcal{S}_n} E^Z_n(\boldsymbol{R}).$$

Proof. Since the case of $n = 1$ is trivial, we assume $n \ge 2$. From (2.8) and (2.17), we only need to prove that there exists an $\boldsymbol{R}^* = (r^*_1, \ldots, r^*_n) \in \mathcal{N}^n_Z$ such that

$$E^Z_n(\boldsymbol{R}^*) = \inf_{\boldsymbol{R}\in\mathcal{N}^n_Z} E^Z_n(\boldsymbol{R}) = \mu^Z_n.$$

Let $\{\boldsymbol{R}_m\} \subset \mathcal{N}^n_Z$ be a minimizing sequence such that $E^Z_n(\boldsymbol{R}_m) \to \mu^Z_n$ as $m \to \infty$. We first show that $\{\boldsymbol{R}_m\}$ is bounded.

Suppose $\{\boldsymbol{R}_m\}$ is unbounded. Let $\boldsymbol{R}_m = (\boldsymbol{r}^m_1, \ldots, \boldsymbol{r}^m_n)$. By replacing $\{\boldsymbol{R}_m\}$ with its subsequence, if necessary, essentially two cases need to be considered:

(a) $|\boldsymbol{r}^m_k| \to +\infty$, $1 \le k \le n$; and

(b) there exist $M > 0$ and k_0: $1 \le k_0 \le n-1$, such that

$$\begin{cases} r^m_k \to +\infty, & 1 \le k \le k_0, \\ r^m_k \le M, & k_0 + 1 \le k \le n. \end{cases}$$

In general, the index set $\{1, 2, \ldots, n\}$ has two disjoint subsets such that $r_k^m \to \infty$ and $r_k^m < M$, respectively, as $m \to \infty$ for k in each of these two index subsets. But the proof is the same.

For case (a), since $\{\mathbf{R}_m\} \subset \mathcal{N}_Z^n$ and (2.18), we have

$$\mu_n^Z = \lim_{m\to\infty} E_n^Z(\boldsymbol{R}_m) = \lim_{m\to\infty} \left\{ -\frac{1}{2} \sum_{i=1}^{n} \frac{n_i^2}{r_i^m} \right\} = 0.$$

This contradicts $\mu_n^Z < 0$ from (2.8). Thus, case (a) is impossible.

For case (b), we can further assume that $\boldsymbol{r}_k^m \to \boldsymbol{r}_k^*$ for $k_0 + 1 \le k \le n$. Then we have

$$\begin{aligned}
\mu_n^Z &= \lim_{m\to\infty} E_n^n(\boldsymbol{R}_m) \\
&= \lim_{m\to\infty} \left\{ \sum_{i=1}^{n} \left(\frac{n_i^2}{2(r_i^m)^2} - \frac{Z}{r_i^m} \right) + \sum_{\substack{i,j=1 \\ i\neq j}}^{n} \frac{1}{2r_{ij}^m} \right\} \\
&= \left\{ \sum_{k=k_0+1}^{n} \left[\frac{n_k^2}{2(r_k^*)^2} - \frac{Z}{r_k^*} \right] + \sum_{\substack{j,k=k_0+1 \\ j\neq k}}^{n} \frac{1}{2r_{jk}^*} \right\} + \lim_{m\to\infty} \sum_{\substack{j,k=1 \\ j\neq k}}^{k_0} \frac{1}{2r_{jk}^m} \\
&\ge \mu_{n-k_o}^Z + \lim_{m\to\infty} \sum_{\substack{j,k=1 \\ j\neq k}}^{k_0} \frac{1}{2r_{jk}^m} \ge \mu_{n-k_0}^Z,
\end{aligned}$$

By applying the first part of Lemma 2, we must have

$$\lim_{m\to\infty} \sum_{\substack{j,k=1 \\ j\neq k}}^{k_0} \frac{1}{r_{jk}^m} = 0,$$

and

$$\mu_n^Z = \mu_{n-k_0}^Z = \sum_{k=k_0+1}^{n} \left[\frac{n_i^2}{2(r_k^*)^2} - \frac{Z}{r_k^*} \right] + \sum_{\substack{j,k=k_0+1 \\ j\neq k}}^{n} \frac{1}{2r_{jk}^*},$$

which contradicts the second part of Lemma 2. Thus, case (b) is also impossible.

Therefore $\{\boldsymbol{R}_m\}$ is bounded and contains a convergent subsequence, denoted by $\{\boldsymbol{R}_m\}$ again, such that $\boldsymbol{R}^m \to \boldsymbol{R}^* \in \mathbb{R}^{3n}$. Since $\mathcal{N}_Z^n$ is a closed subset of $\mathbb{R}^{3n}$, we have $\boldsymbol{R}^* \in \mathcal{N}_Z^n$, and

$$E_n^n(\boldsymbol{R}^*) = \mu_n^Z = \inf_{\boldsymbol{R}\in\mathbb{R}^{3n}\setminus\mathcal{S}_n} E_n^Z(\boldsymbol{R}).$$

□

Corollary 2. *Let $Z = n$. For any nontrivial subspace V of $\mathbb{R}^3$, the energy function E_n^Z defined in (2.1) attains a minimum in V^n.* □

3 Critical Points of the Energy E: Stable and Unstable Electron Configurations

From here throughout the rest of the paper for all practical interest we assume $n = Z$ for E_n^Z, which will be written simply as E.

In order to distinguish any global (or, possibly local) minimizer $\boldsymbol{R}^*$ from a saddle-type critical point $\boldsymbol{R}^\wedge$ of E, we need to examine whether the $(3Z) \times (3Z)$ Hessian matrix D^2E (cf. (2.9)) is (semi-) positive-definite at $\boldsymbol{R}^*$, as the second order Taylor approximation gives

$$\begin{aligned} E(\boldsymbol{R}) &= E(\boldsymbol{R}^*) + DE(\boldsymbol{R}^*) \cdot (\boldsymbol{R} - \boldsymbol{R}^*) + \frac{1}{2}(\boldsymbol{R} - \boldsymbol{R}^*)^T \cdot D^2E(\boldsymbol{R}^*) \cdot (\boldsymbol{R} - \boldsymbol{R}^*) \\ &\quad + \mathcal{O}(|\boldsymbol{R} - \boldsymbol{R}^*|^3) \\ &= E(\boldsymbol{R}^*) + \frac{1}{2}(\boldsymbol{R} - \boldsymbol{R}^*)^T \cdot D^2E(\boldsymbol{R}^*) \cdot (\boldsymbol{R} - \boldsymbol{R}^*) + \mathcal{O}(|\boldsymbol{R} - \boldsymbol{R}^*|^3), \\ &\quad \text{for } |\boldsymbol{R} - \boldsymbol{R}^*| \text{ small,} \end{aligned}$$

requiring that

$$\begin{aligned} &\boldsymbol{R}^T \cdot D^2E(\boldsymbol{R}^*) \cdot \boldsymbol{R} \geq 0 \quad \text{for any} \quad \boldsymbol{R} \in \mathbb{R}^{3Z}, \\ &\text{for } \boldsymbol{R}^* \text{ to be a local or global minimum.} \end{aligned}$$

Following the terminology of calculus of variations, we say that a critical point $\boldsymbol{R}^\wedge$ is *nondegenerate* if $D^2_{\boldsymbol{R}}E(\boldsymbol{R}^\wedge)$ is an invertible (i.e., nonsingular) $(3Z) \times (3Z)$ matrix. Otherwise, $\boldsymbol{R}^\wedge$ is said to be a *degenerate* critical point. Thus, a critical point is degenerate if and only if $D^2_{\boldsymbol{R}}E(\boldsymbol{R}^\wedge)$ has 0 as its eigenvalue. At a critical point $\boldsymbol{R}^\wedge$, the number of negative eigenvalues is called the *Morse index* of that critical point. If a critical point $\boldsymbol{R}^\wedge$ is non-degenerate and has a Morse index greater than or equal to 1, then $\boldsymbol{R}^\wedge$ must correspond to a saddle point of $E(\boldsymbol{R})$. But here all the critical points are degenerate according to the following.

Theorem 3 (Degeneracy of critical points). *Any critical point $\boldsymbol{R}^\wedge$ of $E(\boldsymbol{R})$ is degenerate. The dimension of degeneracy is at least 2.*

Proof. Any critical point $\boldsymbol{R}_0^\wedge$ satisfies (2.10) and, according to Theorem 1, $\mathcal{R}\boldsymbol{R}^\wedge$ is also a critical point for any 3-D rotation $\mathcal{R}$:

$$DE(\mathcal{R}\boldsymbol{R}_0^\wedge) = \boldsymbol{0} \in \mathbb{R}^{3Z}. \tag{3.1}$$

From the theory of Lie groups in $\mathbb{R}^3$, we know that the rotation group $SO(3)$ (i.e., the special orthogonal group) in $\mathbb{R}^3$ can be parametrized by two independent parameters (θ_1, θ_2). So we may write $\mathcal{R} = \mathcal{R}(\theta_1, \theta_2)$ and define

$$\boldsymbol{R}^\wedge(\theta_1, \theta_2) \equiv \mathcal{R}(\theta_1, \theta_2)\boldsymbol{R}_0^\wedge. \tag{3.2}$$

Then by (3.1),

$$DE(\boldsymbol{R}^\wedge(\theta_1, \theta_2)) = \boldsymbol{0} \quad \text{for all} \quad \theta_1 \text{ and } \theta_2. \tag{3.3}$$

Thus, by the chain rule,

$$\frac{\partial}{\partial \theta_j} DE(\boldsymbol{R}^\wedge(\theta_1, \theta_2)) = D^2E(\boldsymbol{R}^\wedge(\theta_1, \theta_2)) \cdot \left[\frac{\partial}{\partial \theta_j}\boldsymbol{R}^\wedge(\theta_1, \theta_2)\right] = \boldsymbol{0}, \qquad j = 1, 2. \tag{3.4}$$

Since

$$\frac{\partial}{\partial \theta_j}\boldsymbol{R}^\wedge(\theta_1, \theta_2) \neq \boldsymbol{0} \quad \text{for} \quad j = 1, 2, \tag{3.5}$$

and $\frac{\partial}{\partial\theta_1}\boldsymbol{R}^\wedge(\theta_1,\theta_2)$ and $\frac{\partial}{\partial\theta_2}\boldsymbol{R}^\wedge(\theta_1,\theta_2)$ are linearly independent, because by holding $\theta_1=\theta_1^0$ and $\theta_2=\theta_2^0$, $\boldsymbol{R}^\wedge(\theta_1,\theta_2^0)$ and $\boldsymbol{R}^\wedge(\theta_1^0,\theta_2)$ form two independent trajectories when only one of θ_1 and θ_2 is allowed to vary, and $\frac{\partial}{\partial\theta_1}\boldsymbol{R}^\wedge(\theta_1,\theta_2^0)$ and $\frac{\partial}{\partial\theta_2}\boldsymbol{R}^\wedge(\theta_1^0,\theta_2)$ are the tangent vectors along these two independent trajectories. We conclude from (3.4) that the Hessian matrix $D^2E(\boldsymbol{R}^\wedge)$ has two linearly independent eigenvectors corresponding to the eigenvalue 0. The proof is complete. □

The determination of *all* critical point $\boldsymbol{R}^\dagger$ from either (2.11) or analytically is no easy task. The following two theorems provide a systematic way to construct (unstable) saddle-type critical points which are not global minima.

Define a subset $\mathbb{R}^{3Z}_x$ of $\mathbb{R}^{3Z}$ by

$$\mathbb{R}^{3Z}_x=\{\boldsymbol{R}=(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_Z)\in\mathbb{R}^{3Z}\mid \boldsymbol{r}_j=(x_j,y_j,z_j)^T=(x_j,0,0),\ \text{for } j=1,2,\ldots,Z;\\ x_j\in\mathbb{R}\}. \tag{3.6}$$

So $\mathbb{R}^{3Z}_x$ is a Z-dimensional subspace of $\mathbb{R}^{3D}$. The subspaces $\mathbb{R}^{3Z}_y$ and $\mathbb{R}^{3Z}_z$ can be defined likewise.

Theorem 4. *The minimization problem*

$$\min_{\boldsymbol{R}\in\mathbb{R}^{3Z}_x} E(\boldsymbol{R}) \tag{3.7}$$

has at least a (global) minimizer $\boldsymbol{R}^*_x\in\mathbb{R}^{3Z}_x$. This $\boldsymbol{R}^*_x$ is also a critical point of E in $\mathbb{R}^{3Z}$, i.e., $DE(\boldsymbol{R}^*_x)=\boldsymbol{0}$. In fact, any critical point $\boldsymbol{R}^\dagger_x$ of $E(\boldsymbol{R})$ in $\mathbb{R}^{3Z}_x$ is also a critical point of E in $\mathbb{R}^{3Z}$, i.e., $DE(\boldsymbol{R}^\dagger_x)=\boldsymbol{0}$. The same is true if $\mathbb{R}^{3Z}_x$ is replaced by $\mathbb{R}^{3Z}_y$ or $\mathbb{R}^{3Z}_z$.

Proof. Because $\mathbb{R}^{3Z}_x$ is a closed subspace of $\mathbb{R}^{3Z}$, we can establish that (3.7) has a minimizer $\boldsymbol{R}^*_x$ in $\mathbb{R}^{3Z}_x$ by Corollary 2. The same conclusion follows for $\mathbb{R}^{3Z}_y$ and $\mathbb{R}^{3Z}_y$.

We now show how $\boldsymbol{R}^*_x$ satisfies $DE(\boldsymbol{R}^*_x)=\boldsymbol{0}$. Since $\boldsymbol{R}^*_x$ solves (3.7), we have the gradient equations

$$\frac{\partial}{\partial x_j}E(\boldsymbol{R})|_{\boldsymbol{R}=\boldsymbol{R}^*_x}=0,\ \text{for } j=1,2,\ldots,Z;\ \text{cf. (3.6) for } x_j.$$

The above gives

$$\left(\frac{n_j^2}{x_j^{*4}}-\frac{Z}{x_j^{*3}}+\sum_{\substack{k=1\\k\neq j}}^{Z}\frac{1}{2|x_k^*-x_j^*|^3}\right)x_j^*-\sum\frac{1}{2|x_k^*-x_j^*|^3}x_k^*=0,\quad j=1,2,\ldots,Z, \tag{3.8}$$

where x_j^*'s are the first components of $\boldsymbol{r}_j^*$, with $\boldsymbol{R}^*_x=(\boldsymbol{r}_1^*,\boldsymbol{r}_2^*,\ldots,\boldsymbol{r}_Z^*)$.

Note that (3.8) just represents the first component (i.e., related to x) of the vector equations (2.12), with "†" therein replaced by "∗". But the second and third components (related to y and z) are automatically satisfied because $y_j=z_j=0$ for $j=1,2,\ldots,Z$. □

Next, define the following subsets of $\mathbb{R}^{3Z}$:

$$\mathbb{R}^{3Z}_{x,y}=\{\boldsymbol{R}=(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_Z)\in\mathbb{R}^{3Z}\mid \boldsymbol{r}_j=(x_j,y_j,z_j)=(x_j,y_j,0),\ \text{for } j=1,2,\ldots,Z;\\ x_j,y_j\in\mathbb{R}\},$$

$$\mathbb{R}^{3Z}_{x,z}=\{\boldsymbol{R}=(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_z)\in\mathbb{R}^{3Z}\mid \boldsymbol{r}_j=(x_j,y_j,z_j)=(x_j,0,z_j),\ \text{for } j=1,2,\ldots,Z;\\ x_j,z_j\in\mathbb{R}\},$$

$$\mathbb{R}^{3Z}_{y,z}=\{\boldsymbol{R}=(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_Z)\in\mathbb{R}^{3Z}\mid \boldsymbol{r}_j=(x_j,y_j,z_j)=(0,y_j,z_j),\ \text{for } j=1,2,\ldots,Z;\\ y_j,z_j\in\mathbb{R}\}.$$

Theorem 5. *The minimization problem*

$$\min_{\boldsymbol{R}\in\mathbb{R}^{3Z}_{x,y}} E(\boldsymbol{R})$$

has at least a (global) minimizer $\boldsymbol{R}^*_{x,y} \in \mathbb{R}^{3Z}_{x,y}$. *This* $\boldsymbol{R}^*_{x,y}$ *is a critical point of* $E(\boldsymbol{R})$ *in* $\mathbb{R}^{3Z}$, *i.e.,* $DE(\boldsymbol{R}^*_{x,y}) = \boldsymbol{0}$. *In fact, any critical point* $\boldsymbol{R}^\dagger_{x,y}$ *of* $E(\boldsymbol{R})$ *in* $\mathbb{R}^{3Z}_{x,y}$ *is also a critical point of* $E(\boldsymbol{R})$ *in* $\mathbb{R}^{3Z}$, *i.e.,* $DE(\boldsymbol{R}^\dagger_{x,y}) = \boldsymbol{0}$. *The same theorem holds if we replace* $\mathbb{R}^{3D}_{x,y}$ *above by* $\mathbb{R}^{3D}_{x,z}$ *or* $\mathbb{R}^{3D}_{y,z}$.

Proof. Same as that for Theorem 4. □

Corollary 3. *Let* V *be a (coordinate) subspace of* $\mathbb{R}^3$ *with dimension 1 or 2. Then any critical point of* E *on* V^Z *is a critical point of* E *on* $\mathbb{R}^{3Z}$.

Proof. Any such V can be obtained by a rotation from $\mathbb{R}^{3Z}_x$ or $\mathbb{R}^{3Z}_{x,y}$, respectively, if V has dimension of, respectively, 1 and 2. The corollary follows because E is rotationally invariant. □

With the aid of Theorems 4 and 5, we will be able to obtain many unstable critical points of $E(\boldsymbol{R})$ in $\mathbb{R}^{3Z}$. See Examples 2 and 3 in Section 5.

We conjecture that the energy function E as defined in (1.5)–(1.10) has only finitely many critical points $\boldsymbol{R}^\dagger$ satisfying $DE(\boldsymbol{R}^\dagger) = \boldsymbol{0}$, which are not rotationally equivalent. But we don't yet have a proof.

4 Coplanarity of Stable or Unstable Electron Configurations

Numerical results (see Example in Section 5) indicate that for $Z = 3$ and 4, the stable electron configuration (corresponding to a global minimizer of E) has all electrons coplanar with the origin. For $Z = 1$ and 2, the coplanarity is trivial. For $Z \geq 5$, numerical evidence suggests that coplanarity no longer holds.

Theorem 6 (Co-planarity of the electrons with the origin: $Z = 3$). *Let* $Z = 3$. *If* $\boldsymbol{R}^\dagger = (\boldsymbol{r}^\dagger_1, \boldsymbol{r}^\dagger_2, \boldsymbol{r}^\dagger_3)$ *is a critical point of* $E(\boldsymbol{R})$ *(including the global minimizer* $\boldsymbol{R}^*$*), then* $\boldsymbol{r}^\dagger_1, \boldsymbol{r}^\dagger_2, \boldsymbol{r}^\dagger_3$, *and* $\boldsymbol{0}$ *are coplanar in* $\mathbb{R}^3$.

Proof. For clarity, we write out the system of equations (2.12):

$$\left.\begin{aligned}
&\left(\frac{1}{r_1^{\dagger 4}} - \frac{3}{r_1^{\dagger 3}} + \frac{1}{r_{12}^{\dagger 3}} + \frac{1}{r_{13}^{\dagger 3}}\right)\boldsymbol{r}^\dagger_1 - \frac{1}{r_{12}^{\dagger 3}}\boldsymbol{r}^\dagger_2 - \frac{1}{r_{13}^{\dagger 3}}\boldsymbol{r}^\dagger_3 = \boldsymbol{0},\\
&\left(\frac{1}{r_2^{\dagger 4}} - \frac{3}{r_2^{\dagger 3}} + \frac{1}{r_{12}^{\dagger 3}} + \frac{1}{r_{23}^{\dagger 3}}\right)\boldsymbol{r}^\dagger_2 - \frac{1}{r_{12}^{\dagger 3}}\boldsymbol{r}_1 - \frac{1}{r_{23}^{\dagger 3}}\boldsymbol{r}^\dagger_3 = \boldsymbol{0},\\
&\left(\frac{4}{r_3^{\dagger 4}} - \frac{3}{r_3^{\dagger 3}} + \frac{1}{r_{13}^{\dagger 3}} + \frac{1}{r_{23}^{\dagger 3}}\right)\boldsymbol{r}^\dagger_3 - \frac{1}{r_{13}^{3}}\boldsymbol{r}^\dagger_1 - \frac{1}{r_{23}^{\dagger 3}}\boldsymbol{r}^\dagger_2 = \boldsymbol{0}.
\end{aligned}\right\} \tag{4.1}$$

If any single equation in (4.1) has all 3 coefficients of $\boldsymbol{r}^\dagger_1, \boldsymbol{r}^\dagger_2$ and $\boldsymbol{r}^\dagger_3$ to be nonzero, then any one vector in $\{\boldsymbol{r}^\dagger_1, \boldsymbol{r}^\dagger_2, \boldsymbol{r}^\dagger_3\}$ can be expressed as a linear combination of the other two vectors, and thus the proof follows. Therefore, the only possibility that $\boldsymbol{r}^\dagger_1, \boldsymbol{r}^\dagger_2, \boldsymbol{r}^\dagger_3$ and $\boldsymbol{0}$ are not coplanar is when

$$\frac{n_i^2}{r_i^{\dagger 4}} - \frac{3}{r_i^{\dagger 3}} - \sum_{\substack{j\neq i\\ j=1}}^{3} \frac{1}{r^\dagger_{ij}} = 0, \quad \text{for} \quad i = 1, 2, 3. \tag{4.2}$$

But the above implies, from (4.2), that

$$\left.\begin{aligned}
\frac{1}{r_{12}^{\dagger 3}}\boldsymbol{r}_2^\dagger + \frac{1}{r_{13}^{\dagger 3}}\boldsymbol{r}_3^\dagger = \mathbf{0}, \\
\frac{1}{r_{12}^{\dagger 3}}\boldsymbol{r}_1^\dagger + \frac{1}{r_{23}^{\dagger 3}}\boldsymbol{r}_3^\dagger = \mathbf{0}, \\
\frac{1}{r_{12}^{\dagger 3}}\boldsymbol{r}_1^\dagger + \frac{1}{r_{23}^{\dagger 3}}\boldsymbol{r}_2^\dagger = \mathbf{0},
\end{aligned}\right\}$$

Adding up the three equations in (4.2), we have

$$\sum_{i=}^{3}\left(\sum_{\substack{j=1\\ j\neq i}}^{3}\frac{1}{r_{ij}^{\dagger 3}}\right)\boldsymbol{r}_i^\dagger = \mathbf{0}.$$

Once again, any $\boldsymbol{r}_i^\dagger$ can be expressed as a linear combination of $\boldsymbol{r}_j^\dagger$ for $j \neq i$. Therefore, $\boldsymbol{r}_1^\dagger, \boldsymbol{r}_2^\dagger, \boldsymbol{r}_3^\dagger$ and $\mathbf{0}$ are coplanar. □

At this time, we are not yet able to prove the coplanarity property for the case $Z = 4$, which as Fig. 3 in the next section indicates, is true from numerical computation.

5 Numerical Examples and Data

We first list in Table 2 the comparison between the experimental values of atoms' ground-state energies and those of the Bohr energies, for atom numbers between 2 and 30. There is a reasonable agreement between these values when Z is small. When the value of Z increases, the deviations also grow. Nevertheless, the *trend* of Bohr's atom energies look good.

Z	Experimental	Bohr's
2.0	−2.903	−3.0615
3.0	−7.478	−7.6889
4.0	−14.667	−14.8377
5.0	−24.652	−24.7906
6.0	−37.842	−37.8128
7.0	−54.584	−54.1540
8.0	−75.059	−74.1726
9.0	−99.719	−97.9746
10.0	−128.919	−125.5152
11.0	−162.233	−156.9173
12.0	−200.026	−192.3112
13.0	−242.315	−231.7757
14.0	−289.322	−275.4952
15.0	−341.208	−323.5122
16.0	−398.601	−376.0176
17.0	−460.102	−433.0846
18.0	−527.494	−494.9136
19.0	−599.924	−561.4195

20.0	−677.558	−632.8097
21.0	−760.575	−709.3828
22.0	−849.285	−791.0756
23.0	−943.804	−878.0731
24.0	−1044.315	−970.5907
25.0	−1150.866	−1068.6207
26.0	−1263.483	−1172.1997
27.0	−1382.494	−1281.5093
28.0	−1507.990	−1396.5737
29.0	−1640.123	−1517.7809
30.0	−1779.048	−1644.9630

Table 2. Comparison of ground state energies of atoms' ground-state energies in hartrees (htr) with atom number Z: $2 \le Z \le 30$, between experimental values and Bohr's energies. When Z is small, there is a better agreement, and the trend is basically sound. But none of Bohr's energies are within the *chemical accuracy* of 5 decimal places.

We now provide several examples below to illustrate **stable** as well as **unstable** electron configurations according to Bohr's model.

Example 1 *(Stable electron configurations for the ground state of the Bohr atom model, with* Z: $3 \le Z \le 10$*).* We set up the problem as follows. In order to avoid the 3-D rotational congruence as stated in Theorem 1, we fix the direction of $\boldsymbol{r}_1$ along the positive z-axis and that of $\boldsymbol{r}_2$ on the (x, z)-plane, as follows:

$$\begin{cases} \boldsymbol{r}_1 = r_1 \boldsymbol{k}, \\ \boldsymbol{r}_2 = r_2 \sin\theta_2 \boldsymbol{i} + r_2 \cos\theta_2 \boldsymbol{k}, \\ \boldsymbol{r}_i = r_i \sin\theta_i \cos\phi_i \boldsymbol{i} + r_i \sin\theta_i \sin\phi_i \boldsymbol{j} + r_i \cos\theta_i \boldsymbol{k}, & i \ge 3, \\ 0 \le \theta_i \le \pi, \quad 0 \le \phi_i \le 2\pi, & i \ge 2. \end{cases} \tag{5.1}$$

Then the relative distances become

$$\begin{cases} r_{1i} = (r_1^2 - r_i^2 - 2r_1 r_i \cos\theta_i)^{1/2}, & 2 \le i \le Z, \\ r_{2i} = [r_2^2 + r_i^2 - 2r_2 r_i (\sin\theta_2 \sin\theta_i \cos\phi_i + \cos\theta_2 \cos\phi_i)]^{1/2}, & 3 \le i \le Z, \\ r_{ij} = [r_i^2 + r_j^2 - 2r_i r_j (\sin\theta_i \sin\theta_j \cos(\phi_i - \phi_j) + \cos\theta_i \cos\theta_j)]^{1/2}, & 3 \le i < j < Z. \end{cases} \tag{5.2}$$

The stable electron configurations corresponding to minimal ground state energy of (1.5) are shown in the next few figures, along with the data given in the captions.

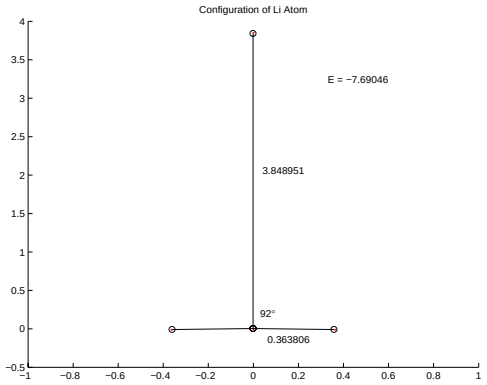


Fig. 2 For lithium (Li), $Z = 3$. The electron configuration is shown above. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.363806, \qquad r_3 = 3.848951,\\
&\theta_2 = 1.605660 = 91.99754143^\circ \neq \frac{\pi}{2},\\
&\theta_3 = 1.605660 = 91.99754131^\circ \neq \frac{\pi}{2}, \phi_3 = \pi,\\
&E = -7.69046(htr); htr = \text{hartree}.
\end{aligned}
$$

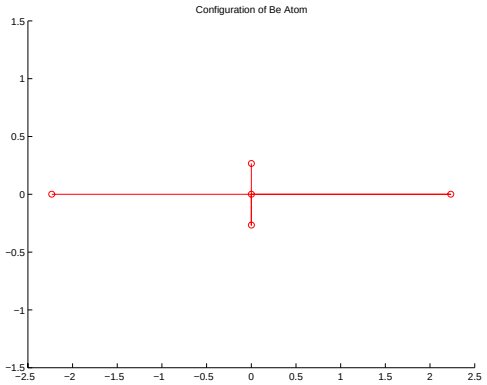


Fig. 3 For beryllium (Be), $Z = 4$. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.26690, \theta_2 = 3.14159 = \pi,\\
&r_3 = r_4 = 2.23196, \theta_3 = \theta_4 = 1.57080 = \frac{\pi}{2}, \phi_3 = \phi_4 = 3.14159 = \pi,\\
&E = -14.84035(htr).
\end{aligned}
$$

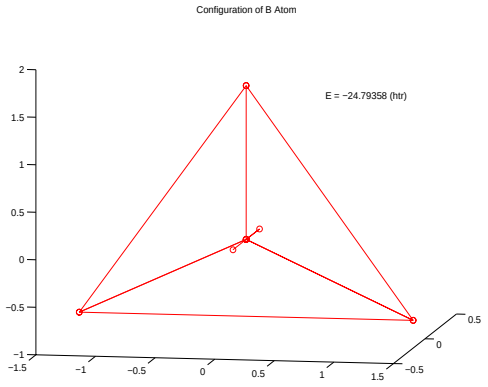


Fig. 4 For boron (B), $Z = 5$. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.21081, r_3 = r_4 = r_5 = 1.61777,\\
&\theta_2 = 2.09440 = \frac{2\pi}{3}, \theta_3 = 2.09440 = \frac{2\pi}{3}, \phi_3 = 3.14159 = \pi,\\
&\theta_4 = 1.57080 = \frac{\pi}{2}, \phi_4 = 1.57080 = \frac{\pi}{2},\\
&\theta_5 = 1.57080 = \frac{\pi}{2}, \phi_5 = -1.57080 = -\frac{\pi}{2},\\
&E = -24.79358(htr).
\end{aligned}
$$

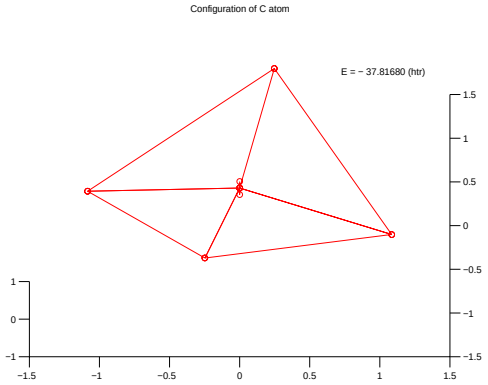


Fig. 5 For carbon (C), $Z = 6$. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.17398, r_3 = r_4 = r_5 = r_6 = 1.29353, \theta_2 = 3.14159 = \pi,\\
&\theta_3 = 2.10638, \phi_3 = -0.22466,\\
&\theta_4 = 1.03522, \phi_4 = 1.34614,\\
&\theta_5 = 2.10638, \phi_5 = 2.91693,\\
&\theta_6 = 1.03522, \phi_6 = -1.79546,\\
&E = -37.81680(htr).
\end{aligned}
$$

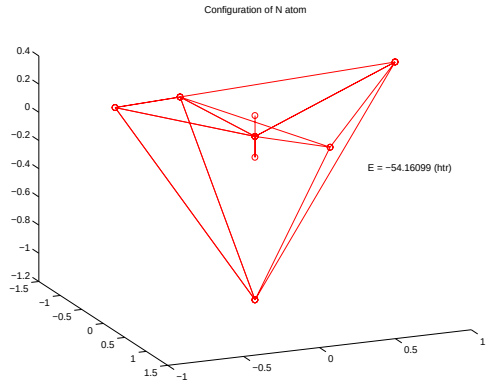


Fig. 6 For nitrogen (N), $Z = 7$. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.14822, r_3 = r_6 = 1.06095, r_4 = r_5 = 1.05175, r_7 = 1.15887,\\
&\theta_2 = 3.14159 = \pi,\\
&\theta_3 = -\theta_6 = 1.21801, \phi_3 = \phi_6 = -0.19528,\\
&\theta_4 = \theta_5 = 1.47408, \phi_4 = 1.37551,\\
&\phi_5 = -1.76608,\\
&\theta_7 = 3.14159 = \pi, \phi_7 = 0.32885,\\
&E = -54.16099(htr).
\end{aligned}
$$

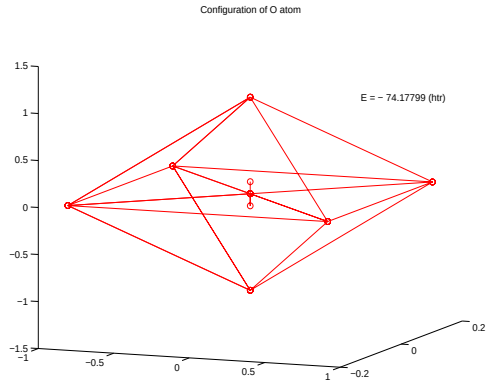


Fig. 7 For oxygen (O), $Z = 8$. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.12910, r_3 = r_4 = r_5 = r_6 = 0.87770, r_7 = r_8 = 1.02674,\\
&\theta_2 = \theta_8 = \pi, \theta_3 = \theta_4 = \theta_5 = \theta_6 = \pi/2, \theta_7 = 0,\\
&\phi_3 = -0.19720, \phi_4 = 1.37360, \phi_5 = 2.94440, \phi_6 = -1.76800, \phi_7 = -0.48203, \phi_8 = -0.73723,\\
&E = -74.17799(htr).
\end{aligned}
$$

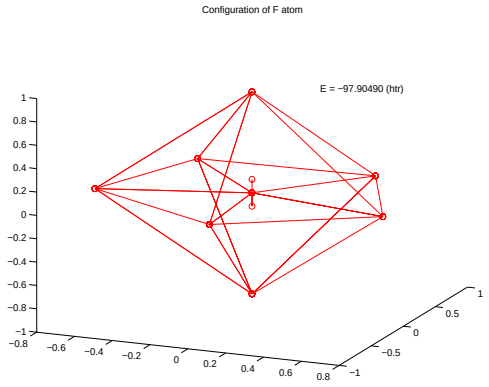


Fig. 8 For fluorine (F), $Z = 9$. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.11435, r_3 = r_4 = r_5 = r_6 = r_7 = 0.78823, r_8 = r_9 = 0.86558,\\
&\theta_2 = \theta_9 = \pi, \theta_3 = \theta_4 = \theta_5 = \theta_6 = \theta_7 = \pi/2, \theta_8 = 0,\\
&\phi_3 = -0.26152, \phi_4 = 0.99512, \phi_5 = 2.25176, \phi_6 = 3.50839, \phi_7 = 4.76503, \phi_8 = -0.21356,\\
&\phi_9 = -0.02196,\\
&E = -97.90490(htr).
\end{aligned}
$$

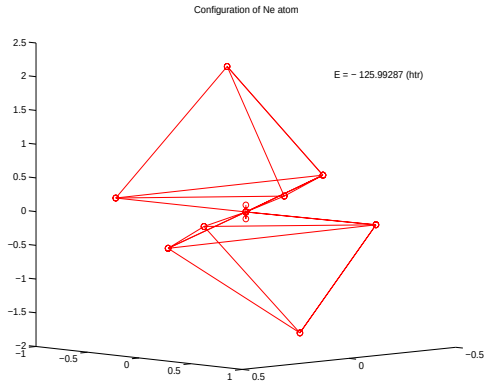


Fig. 9 For neon (NE), $Z = 10$. We have

$$
\begin{aligned}
&r_1 = r_2 = 0.10263, r_3 = 2.14617, r_4 = 0.63726, r_5 = 0.63288, r_6 = 0.63387,\\
&r_7 = 0.63355, r_8 = 0.63008, r_9 = 0.62496, r_{10} = 1.87083,\\
&\theta_2 = 3.13987(\neq \pi), \theta_3 = -0.06317, \theta_4 = 0.99093, \theta_5 = 1.06946, \theta_6 = 0.98591, \theta_7 = 2.13822,\\
&\theta_8 = 2.11486, \theta_9 = 2.04094, \theta_{10} = 3.01675,\\
&\phi_3 = -0.16895, \phi_4 = 0.14127, \phi_5 = 2.17293, \phi_6 = 4.25346, \phi_7 = 1.11058, \phi_8 = 3.25805,\\
&\phi_9 = -0.94826, \phi_{10} = -1.32532,\\
&E = -125.99287(htr).
\end{aligned}
$$

Example 2 *(Saddle-type unstable colinear electron configurations, $Z = 3$).* Consider the case of Li, $Z = 3$. Write

$$
\begin{cases}
\boldsymbol{r}_3 = r_3\boldsymbol{k}, \boldsymbol{r}_1 = r_1 \sin\theta_1\boldsymbol{i} + r_1\cos\theta_1\boldsymbol{k},\\
\boldsymbol{r}_2 = r_2\cos\theta_2\boldsymbol{k} + r_2\sin\theta_2\cos\phi_2\boldsymbol{i} + r_2\sin\theta_2\sin\phi_2\boldsymbol{j}.
\end{cases}
\tag{5.3}
$$

We consider

$$\min_{\boldsymbol{R}\in\mathbb{R}^9_z} E(\boldsymbol{R}), \quad \boldsymbol{R}=(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)=\left(\begin{bmatrix}0\\0\\r_1\end{bmatrix},\begin{bmatrix}0\\0\\r_2\end{bmatrix},\begin{bmatrix}0\\0\\r_3\end{bmatrix}\right), \tag{5.4}$$

i.e., all 3 vectors $\boldsymbol{r}_1,\boldsymbol{r}_2$ and $\boldsymbol{r}_3$ are required to be colinear on the z-axis. This can be done by setting $\phi_2=\pi$ and by requiring θ_1 and θ_2 to be equal to either 0 or π in (5.3).

For problem (5.4), we have found 5 critical points $\boldsymbol{R}_i^\dagger$, $i=1,2,3,4,5$, with respect to the 3 scalar variables r_1,r_2 and r_3. See Table 3 below.

critical points	coordinates (cf. (5.3)) (set $\phi_2=\pi$)					Energies
	r_1	r_2	r_3	θ_1	θ_2	
$\boldsymbol{R}_1^\dagger$	1.0334	0.3133	7.2778	0	0	−5.5985
$\boldsymbol{R}_2^\dagger$	0.3622	0.3647	4.1865	0	π	−7.6837
$\boldsymbol{R}_3^\dagger$	0.3647	0.3622	4.1865	π	0	−7.6837
$\boldsymbol{R}_4^\dagger$	1.0967	0.3174	2.2462	π	π	−5.7752
$\boldsymbol{R}_5^\dagger$	0.3174	1.0967	2.2462	π	π	−5.7752

Table 3 Locations of four critical points of problem (5.4). Note that only $\boldsymbol{R}_2^\dagger$ and $\boldsymbol{R}_3^\dagger$ are true minimizers for (5.4), while $\boldsymbol{R}_1^\dagger$, $\boldsymbol{R}_4^\dagger$ and $\boldsymbol{R}_5^\dagger$ are just local minima for (5.4).

Note that by Theorem 4, all these points $\boldsymbol{R}_i^\dagger$, $i=1,2,3,4,5$, are critical points of E on $\mathbb{R}^{3Z}$. On the other hand, fix $\phi_2=\pi$ only. Then $\boldsymbol{r}_1,\boldsymbol{r}_2$ and $\boldsymbol{r}_3$ are coplanar and

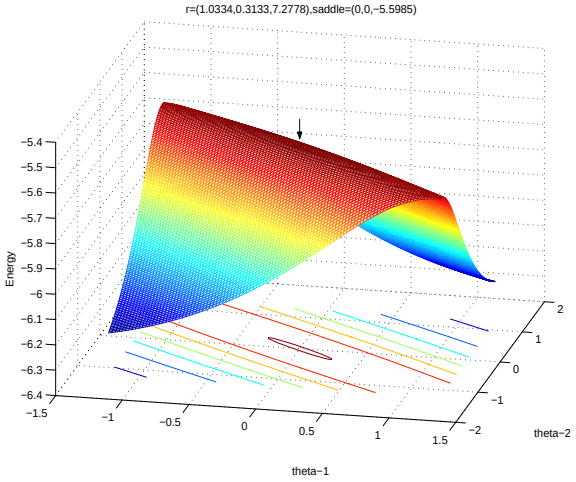
$$\begin{aligned} E(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) &= \frac{1}{2r_1}+\frac{1}{2r_2}+\frac{4}{2r_3}-\sum_{i=1}^{3}\frac{3}{r_i}+\left(\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}+\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_3|}+\frac{1}{|\boldsymbol{r}_2-\boldsymbol{r}_3|}\right)\\ &\equiv E(r_1,r_2,r_3,\theta_1,\theta_2). \end{aligned} \tag{5.5}$$

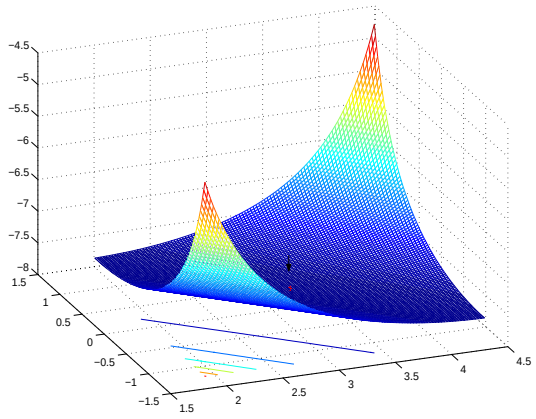
Numerical computations of the Hessian matrix $H=[\partial^2 E/\partial\theta_i\partial\theta_j]_{1\le i,j\le 2}$ and Lemma 1 show that, indeed, these $\boldsymbol{R}_i^\dagger$ are saddle-type critical points. See Table 4.

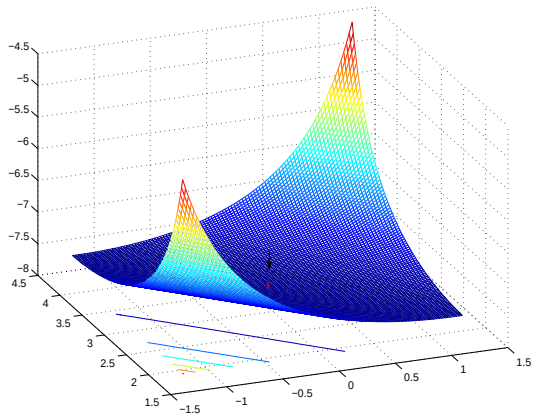
point	two eigenvalues of Hessian $[\partial^2 E/\partial\theta_i\partial\theta_j]$	eigenvectors
$\boldsymbol{R}_1^\dagger$	−1.7530, −0.0187	$(-0.7120,\ -0.7022)^T$, $(0.7022,\ -0.7120)^T$
$\boldsymbol{R}_2^\dagger$	−0.0061, 0.6831	$(-0.7290,\ 0.685)^T$, $(0.6845,\ 0.7290)^T$
$\boldsymbol{R}_3^\dagger$	−0.0061, 0.6831	$(0.6845,\ -0.7290)^T$, $(-0.7290,\ -0.6845)^T$
$\boldsymbol{R}_4^\dagger$	−1.4170, 0.0542	$(0.7014,\ 0.7128)^T$, $(-0.7128,\ 0.7014)^T$
$\boldsymbol{R}_5^\dagger$	−1.4170, 0.0542	$(0.7014,\ 0.7128)^T$, $(-0.7128,\ 0.7014)$

Table 4 Eigenvalues of the Hessian with respect to the angular variables θ_1 and θ_2.

In Fig. 10, we plot the energy surfaces of E with respect to the angular variables θ_1 and θ_2 in a neighborhood of these critical points $\boldsymbol{R}_i^\dagger$.


r=(1.0334,0.3133,7.2778),saddle=(0,0,−5.5985)
Energy
theta−1
theta−2





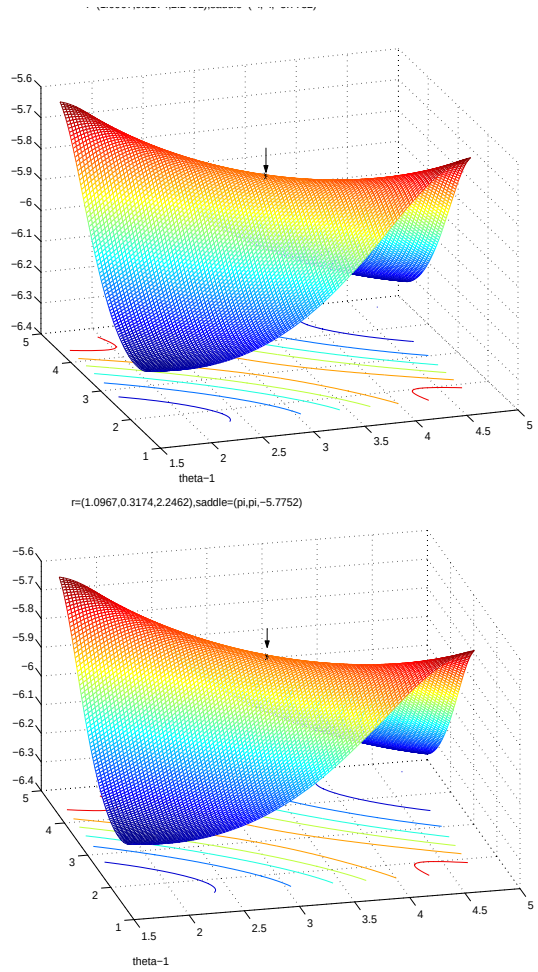


Fig. 10 The energy surface E plotted against the angular variables θ_1 and θ_2 (cf. (5.3)) near the critical points $\boldsymbol{R}_i^\dagger$, $i = 1, 2, 3, 4, 5$, (cf. Table 3) in sequential order, whose locations are pin-pointed by an arrow. These surfaces are all of the saddle type.

It is quite interesting to note from Fig. 2 earlier that the global minimum value of E on $\mathbb{R}^9$ is -7.69046 htr, while the global minimum value of E in (5.4) by restricting all $\boldsymbol{r}_i$, $i = 1, 2, 3$, to lie on the z-axis is -7.6837 htr, (cf. Table 3), which differs from -7.69046 by less than 0.1%. □

Example 3 *(Saddle type unstable coplanar electron configurations, $Z = 5$).* In order to find unstable coplanar electron configurations, Z must be greater than or equal to 5, as Section 4 has proved that $Z = 3$ can only have stable configurations and Fig. 2 has provided a numerical evidence that $Z = 4$ also has stable coplanar electron configurations. For $Z = 5$, we apply Theorem 6 to find coplanar configurations, which must be of the saddle-type and unstable, as Fig. 4 shows that a stable configuration cannot be coplanar. Several unstable configurations can be seen in Fig. 11.

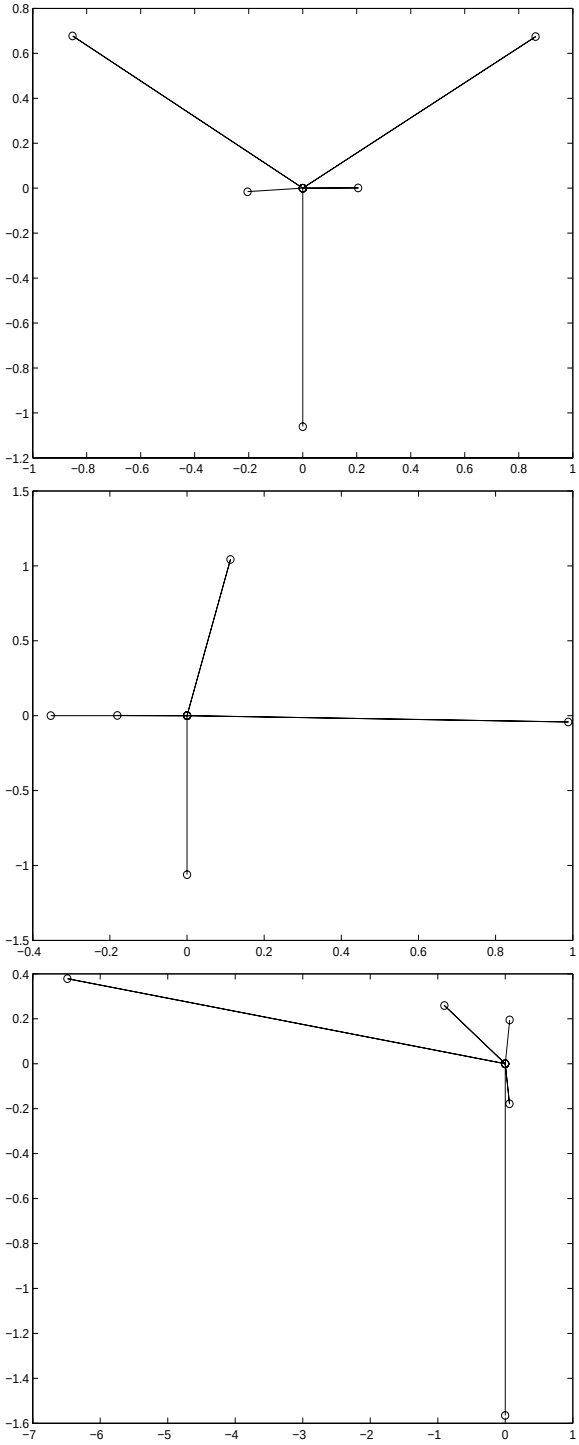


Fig. 11 For $Z = 5$ (boron), the above three configurations are obtained according to Theorem 6 by finding critical points of E on the (x, y)-plane numerically. They should be contrasted with the one in Fig. 4. Coordinates of the five vectors, as well as the corresponding energy values, given

from top to bottom for these three configurations, are:

$(-0.2045, -0.0156, 0), (0.2050, 0.0014, 0), (0.8625, 0.6741, 0), (-0.8524, 0.6777, 0), (0., -1.0604, 0)$
with $E_{\min} = -28.9146$

$(-0.3532, 0, 0), (-0.1808, 0.0011, 0), (0.9884, -0.0419, 0), (0.1128, 1.0034, 0), (0., -1.0610, 0)$
with $E_{\min} = -24.9439$

$(0.0661, 0.1942, 0), (0.0628, -0.1781, 0), (-6.4876, 0.3784, 0), (-0.9024, 0.2594, 0), (0., -1.5647, 0)$
with $E_{\min} = -27.5713$

6 Conclusions

In this paper, we have conducted basic mathematical analysis for existence of minimal energy configurations and certain properties of critical points for the Bohr energy function. Relevant numerical results are also developed and presented.

There are still interesting problems remaining open. One among them is the *coplanarity* of the stable electron configuration for $Z = 4$, which we have not yet been able to prove in Section 4. Also, the determination of the many symmetries manifested in Figs. 2–9 has not been achieved.

Bohr's original model for *molecules* [3] (which generalized the atomic case studied here) had some difficulties which has recently been improved by Svidzinsky, Scully and Hershbach [13]. It has many interesting mathematical features therein worth investigation and we hope to be able to do it in the near future.

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