International Journal of Information Technology and Knowledge Management
July-December 2010, Volume 3, No. 2, pp. 691-694

AUTOMATING THE PROCESS OF FINDING THE ELECTRON CONFIGURATION OF AN ATOM USING FINITE STATE MACHINE

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The Finite State Machine (FSM) designed to automate the process of writing down the electron configuration of an atom of any known element attempts to reduce the complexities faced by researchers, scholars and students involved in the field of atomic physics, specifically dealing with the orientation and arrangement of electrons inside the atom and remembering the exceptional trends in the arrangement of electrons inside the orbitals. This machine takes one electron as input at a time, checks for its best possible transition and places the electron at its required position and orientation inside the orbital. After transition, the output state for each subsequent electron to be filled depends on the experimentally proved factors determined by researchers in the past. This machine also takes into account the exceptions seen in the trends of filling electrons in the orbitals depending upon various stability factors, such as half-filled and completely-filled orbitals, inert pair effect, etc.
Keywords: Electron Configuration, Finite State Machine, Atomic Orbitals.

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1. INTRODUCTION

Finite State Machine: A finite state machine (FSM) or a finite state automaton is a model of behavior composed of a finite number of states, transitions between those states, and actions. It is similar to a “flow graph” where we can inspect the way in which the logic runs when certain conditions are met. A current state is determined by past states of the system. As such, it can be said to record information about the past, i.e., it reflects the input changes from the system start to the present moment. A transition indicates a state change and is described by a condition that would need to be fulfilled to enable the transition. An action is a description of an activity that is to be performed at a given moment. There are several action types:

- Entry Action: Which is performed when entering the state.
- Exit Action: Which is performed when exiting the state
- Input Action: Which is performed depending on present state and input conditions
- Transition Action: Which is performed when performing a certain transition [1].

An FSM can be represented using a state diagram (or state transition diagram) as shown in fig.1, or using a transition table as shown in fig.2.

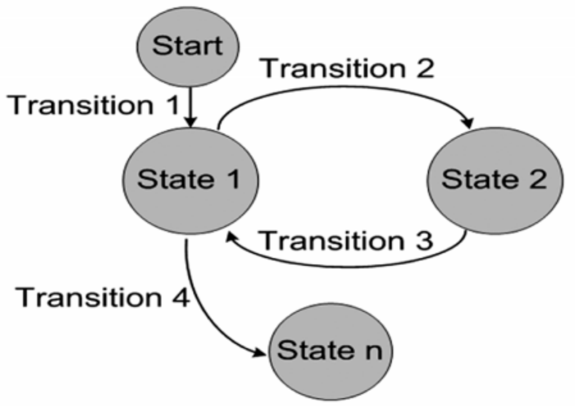

Fig.1: Transition Diagram

Transitions	Current State 1	Current State 2
Condition X	State 2	State 2
Condition Y	State 1	State 1

Fig.2: Transition Table

Electron Configuration: In atomic physics and quantum chemistry, electron configuration is the arrangement of electrons of an atom, a molecule, or other physical structure. It concerns the way electrons can be distributed in the orbitals of the given system.

The electron configuration of an atom is the particular distribution of electrons among available shells. It is described by a notation that lists the sub-shell symbols, one after another. Each symbol has a subscript on the right giving the number of electrons in that sub-shell. For example, a configuration of the lithium atom (atomic number 3) with two electrons in the 1s sub-shell and one electron in the 2s sub-shell is written $1s^2 2s^1$.

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Sub-level	Orbital	maximum no. of electrons
s	1	2
p	3	6
d	5	10
f	7	14

The notation for electron configuration gives the number of electrons in each sub-shell. The number of electrons in an atom of an element is given by the atomic number of that element. The detailed representation of the electron configuration of Helium atom (atomic number 2) is shown in fig.3 [2].

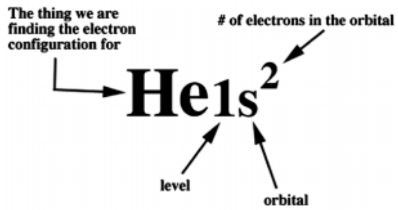

Fig.3: Detailed Representation of Electron Configuration of a Helium Atom

2. RELATED WORK

In the past, there have been lots of developments in the field of quantum chemistry and atomic physics, so as to mechanically or manually solve problems related to the structures of molecules, atoms and the placements and orientation of electrons, protons, neutrons and other basic particles inside an atom.

The Electron Configuration specifically deals with the arrangement of electrons in an atom. Electron configuration was first conceived of under the Bohr model of the atom. An electron shell is the set of allowed states electrons may occupy which share the same principal quantum number, n (the number before the letter in the orbital label). An electron shell can accommodate $2n^2$ electrons, i.e. the first shell can accommodate 2 electrons, the second shell 8 electrons, the third shell 18 electrons, etc. The factor of two arises because the allowed states are doubled due to electron spin—each atomic orbital admits up to two otherwise identical electrons with opposite spin, one with a spin +1/2 (usually noted by an up-arrow) and one with a spin -1/2 (with a down-arrow).

A sub-shell is the set of states defined by a common azimuthal quantum number, l, within a shell. The values l = 0, 1, 2, 3 correspond to the s, p, d, and f labels, respectively. The number of electrons which can be placed in a sub-shell is given by 2(2l + 1). This gives two electrons in an s sub-shell, six electrons in a p sub-shell, ten electrons in a d sub-shell and fourteen electrons in an f sub-shell [5].

Writing down the Electron Configuration of an atom involves the following steps:

a) Find out how many electrons the atom has. On the periodic table, the atomic number is the number of protons of the atom, and thus equals the number of electrons in an atom with zero charge.

b) Refer to fig.4 for a list of orbitals that will hold the electrons.

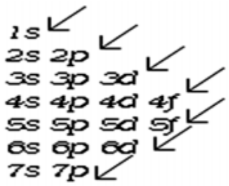

Fig. 4: List of Orbitals

- The s orbital set (any number followed by an "s") contains a single orbital, and by Pauli's Exclusion Principle, a single orbital can hold a maximum of two electrons, so each s orbital set can hold two electrons.
- The p orbital set contains three orbitals, and thus can hold a total of six electrons.
- The d orbital set contains five orbitals, so it can hold ten electrons.
- The f orbital set contains seven orbitals, so it can hold fourteen electrons.

c) Put one electron into the highest energy orbital available, starting with 1s (holds a maximum of two electrons). Fill the orbitals in the order as mentioned (the number following the orbital set is the maximum number of electrons it can hold):

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^6\ 7s^2\ 5f^{14}\ 6d^{10}$

d) Once every electron has been put into an orbital (according to the order), write the configuration as shown at the end of step c, except, write the number of electrons that are in the orbital set instead of the numbers shown (they are shown as completely filled). So, an uncharged sodium atom's electron configuration would be $1s^2\ 2s^2\ 2p^6\ 3s^1$. Notice that the number following 3s isn't 2, but one. That's because only one electron is in the orbital set, so the orbital set is not completely occupied (it lacks one more electron) [6].

These rules are followed by atoms of most of the known elements but not by all. Some exceptions are seen that arise due to one or more reasons. These reasons include higher stability of half-filled and completely-filled orbitals and inert- pair effect, to name a few. Thus, the elements showing exceptional behavior need to be taken care of, each time their structure or electronic arrangement is considered. To avoid this complexity faced by chemical researchers, scholars and students, a finite state machine based system is designed to find out the electron configuration of atoms of any element, taking into account their exceptional behavior and varying trends.

3. PROPOSED WORK

Our main objective behind developing the finite state machine to find out the electronic configuration of any atom is to automate the process of finding the arrangement and orientation of electrons in different orbitals inside an atom of any known element. This system works similar to that of a finite state machine, i.e., it has an input state, a pre-defined transition table, and the output is based on the current state and the current condition. It takes one electron as input at a time, checks for its best possible transition and places the electron at its required position and orientation inside the orbital. After transition, the output state for each subsequent electron to be filled depends on the experimentally proved factors determined by researchers in the past. This machine also takes into account the exceptions seen in the trends of filling electrons in the orbitals depending upon various stability factors, such as half-filled and completely-filled orbitals, inert pair effect, etc [19].

The algorithm involved in designing the mentioned Finite State Machine, which has already been successfully implemented in out project named "INORGANIC EXPERT", is as follows:

```
//Sample code in C#

//here, i is the number of orbital to be filled and atno is the atomic number of the element
for (int i = 0; i < 19 && atno >= 1; i++)
 {
 for (int j = 0; j < elec[i].Length && atno >= 1; j++)
 {
 elec[i][j] = true; //electron is filled at jth
                                   //location of ith orbital
atno—;     //reduce count of electron by one
    //Some exeptional cases
if (i == 6 && j == 3) //atno24,25 half-filled orbitals
 {
 elec[6][4] = true;//electron is filled
 elec[5][1] = false;//electron is not filled
 if (atno >= 1)
 {
 elec[5][1] = true;
 atno—;
 j++;
 }
 }
 if (i == 6 && j == 8) //atno29,30 full-filled orbitals
 {
 elec[6][9] = true;
 elec[5][1] = false;
 if (atno >= 1)
 {
 elec[5][1] = true;
 atno—;
 j++;
 }
 }
 //some other exceptional case, e.g.
 if (i == 12 && j == 0) //atno57 to 63
 {
 elec[13][0] = true;
 elec[12][0] = false;
 if (atno >= 1)
 {
 elec[13][0] = false;
 elec[12][0] = true;
 elec[12][1] = true;
 atno—;
 }

 j++;
 }
// and so on
 }
 }
```

The above code is a sample code to implement the mentioned finite state machine. This code shows only a few exceptions that arise in writing the electron configuration of an element, while the other exceptions have been implemented in a similar fashion, in our project named "INORGANIC EXPERT – automation of Inorganic Chemistry".

4. CONCLUSION AND FUTURE SCOPE

Till date, the filling of electrons inside atomic orbitals as well as the study of their arrangements and orientations is done manually by the chemists, physicists, scholars and students in almost every part of the world. Scarce work is done to automate these processes. Since this system automates almost all of these processes, taking into account the exceptional cases, it defines a good future scope for itself. The machine would be of a great help to everyone involved in the field of atomic physics, as it greatly reduces the overhead of remembering the different rules to fill the orbitals, the varying trends, and the exceptions seen due to various stability factors. It takes the atomic number of the element as the input and provides the user with the electron configuration of the specified element, with the arrangement and orientation if each electron, which can be a quite cumbersome process in case of heavy elements, if done manually. Thus, this system finds its application at various laboratories, research institutions, colleges and schools. Moreover, the machine has been successfully implemented in our project named "INORGANIC EXPERT – automating the Inorganic Chemistry" [9].

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