Automated drawing system of quantum energy levels

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Abstract. The purpose of this work is to derive an automated system that provides advantageous drawings of energy spectra for quantum systems (nuclei, atoms, molecules, etc.) required in various physical sciences. The automation involves the development of appropriate computational code and graphical imaging system based on raw data insertion, theoretical calculations and experimental or bibliographic data insertion. The system determines the appropriate scale to depict graphically with the best possible way in the available space. The presently developed code operates locally and the results are displayed on the screen and can be exported to a PostScript file. We note its main features to arrange and visualize in the available space the energy levels with their identity, taking care the existence in the final diagram the least auxiliary deviations. Future improvements can be the use of Java and the availability on the Internet. The work involves the automated plotting of energy levels in molecules, atoms, nuclei and other types of quantized energy spectra. The automation involves the development of an appropriate computational code and graphical imaging system.

1. Introduction

1.1. Method

This method is based on raw data insertion, theoretical calculations and experimental data insertion or bibliographic data insertion, alone or in a combination of all the methods listed above and the system determines the appropriate scale to depict graphically the best way possible in the available space offered to it. Java has been chosen as the programming language.

NetBeans 7.3.1 IDE (Integrated Development Environment) has been used in order to implement the program. Also JDK (Java Development Kit) version 7u40 as well as JRE (Java Runtime Environment) version 1.7.0. Swing was used in order to implement the user interface. VectorGraphics2D Library used for graphics creation [1]. VectorGraphics2D extends Java.awt.Graphics2D and contains implementations of methods located in Java.awt.Graphics2D [2]. VectorGraphics2D provides the ability to export the graphics in different formats of vector files. The methods which are being used in the implementation of the code are the following: (i) Public abstract void draw(Shape s) and (ii) Public abstract void draw String(String str, int x, int y)

1.1.1. Public abstract void draw(Shape s) Public abstract void draw(Shape s) strokes the outline of a Shape using the settings of the current Graphics2Dcontext.
Parameters: s - the Shape to be rendered. Most of the shapes inserted as a parameter in the
draw operation can be defined by using an additional package which is java.awt.geom. In the
following example we are using java.awt.geom.Line2D which is part of java.awt.geom. In this
specific example we are drawing a line.

```java
import java.awt.Graphics2D;
import java.awt.geom.Ellipse2D;
import java.awt.geom.Line2D;
import java.io.FileOutputStream;
import java.io.IOException;
import de.erichseifert.vectorgraphics2d.EPSGraphics2D;
EPSGraphics2D g = new EPSGraphics2D(0.0,0.0,210.0,297.0);
g.draw(new Line2D.Double(x, 0.0, x, 297.0));
```

1.1.2. public abstract void draw String(String str, int x,int y) Public abstract void draw
String(String str, int x,int y) renders the text of the specified String, using the current text
attribute state in the Graphics2D context. The baseline of the first character is at position (x,
y) in the User Space.
Parameters:
str - the string to be rendered
x - the x coordinate of the location where the String should be rendered
y - the y coordinate of the location where the String should be rendered

VectorGraphics2D provides the ability to export the graphics in different formats of vector
files. More specifically in formats that are more suitable for incorporating them in research
papers such as: (i) Encapsulated PostScript (EPS), (ii) Scalable Vector Graphics (SVG), and
(iii) Portable Document Format (PDF). Using VectorGraphics2D has some inherited restrictions.
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specifically different text encodings are not supported as well as font embedding. We will try
to address these restrictions in a more comprehensive version of this paper. The program’s
features help to arrange and visualize, in the available space, a set of energy levels with their
identity (quantum numbers), in such a way that in the final drawing to appear the least auxiliary
deviations. From the existed programs today, others are very cumbersome due to the complexity
of the input data [3], others have not automated this feature and either manually the researcher
puts the desired deviations [4] or all deviations are only in one direction, usually upwardly [6].

2. Results
The program is user-friendly and the user easily imports the data which are stored to a file. From
the drawings obtained with our code for the excitation spectra of two typical nuclear isotopes
\(^{114}Cd\) and \(^{97}Mo\) illustrated in Figs. 1 and 2, we conclude that our method is very well and
its compared with other methods of automated imaging of energy levels is quite good. Figure 1
shows the representation of the experimental (left panel) and theoretical (right panel) excitation
spectrum of \(^{114}Cd\) isotope while in Fig. 2 we compare two diagrams of the same energy spectrum
(that of \(^{97}Mo\) isotope derived in [6]), one (left panel) obtained with the method of Ref. [6] and
the other from our own code.

One can notice eleven deviations in the plot of Ref. [6] (levels at 0.78, 0.84, 0.93, 1.01, 1.22,
1.40, 1.49, 1.58, 1.60 and 1.60 MeV), while in our plot only six (levels 0.76, 1.40, 1.49, 1.58, 1.60
and 1.60 MeV). Furthermore, the eleven deviations of [6] are upwardly while in our case four are
Figure 1. Experimental (left) and theoretical (right) energy spectrum (in units of MeV) for $^{114}$Cd isotope plotted by using the proposed algorithm. The advantages of the present drawing system are obvious [5].

The energy levels are presented downwardly (at 0.76, 1.40, 1.49, 1.58 MeV) and two (those at 1.60 MeV) upwardly. This means that in our drawing nine energy levels are presented without any deviation while the code used in [6] produces only four levels without deviation.

$^{114}$Cd
Figure 2. Comparison of the energy spectra (in units of MeV) for $^{97}$Mo isotope generated in an automated way in Ref. [6] (left) and the in our new automated code.

We note that, the application of our code on several other diagrams showed us that both the ease of handling as well as the quality of the results are excellent.

3. Conclusions
The code derived in this work is offered for qualitative energy diagrams and can be used by researchers in various disciplines. In the near future the system will be developed by using Java and will be available on the Internet. The interested researcher can enter data directly and receive the charts in the chosen format.

References
[1] VectorGraphic2D Library Home Page http://trac.erichseifert.de/vectorgraphics2d
[2] Graphics2D (Java Platform SE 7 )-Oracle Documentation
   http://docs.oracle.com/javase/7/docs/api/java/awt/Graphics2D.html
[3] Charles L.Dunford, Robert R. Kinsey ENSDAT
   (Evaluated Nuclear Structure Drawings and Tables) Version 12.23 (2007) National Nuclear Data Center
   http://www.nndc.bnl.gov/nndcser/ensdf_gm/utility/ensdat/
[4] M.A. Caprio LevelScheme: A level scheme drawing and scientific figure preparation system for Mathematica
   http://www.sciencedirect.com/science/article/pii/S0010465505002900 - item1-item1 Computer Physics Communications V171, 2, (2005) 107-118.
[5] Tsakstara V, Kosmas T.S Phys. Rev. C, to appear.
[6] Ydrefors E, Mustonen M.T, Suhonen J 2010 Nucl. Phys. A 842 33-47.