UNIVERSIDAD DE GUANAJUATO

What happens if two cats are combined?, gouting the schrödinger's cat with python

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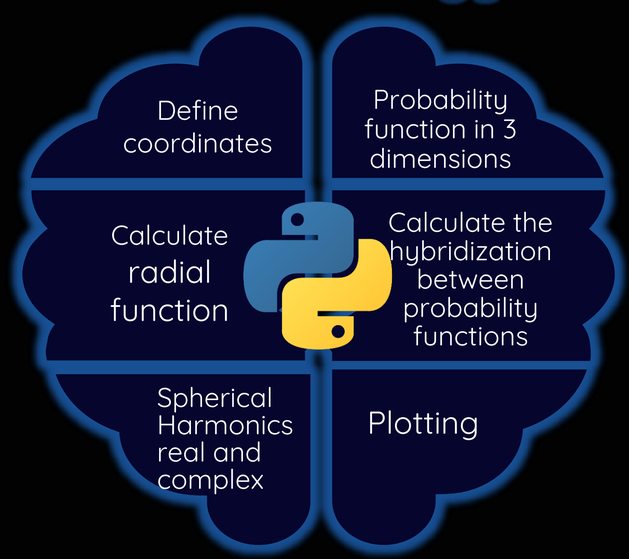
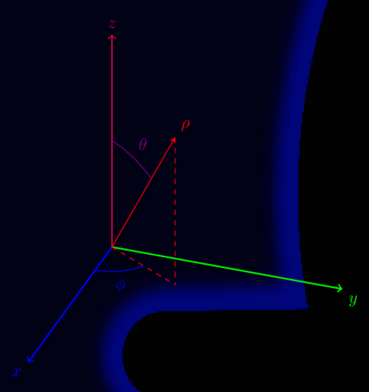
Abstract

In pregrade, students refuse complex topics such as quantum mechanics. Despite that the basic concepts have been introduced often, they are misunderstood due to a lack of good pedagogical resources that may light the topics. An image says more than words, and Chemical model graphics are an intuitive and friendly way to teach students concepts of quantum mechanics; with tools such as Python, we can teach them simple and attractive for the student. The following work will show the beauty of the area with interactive plots generated with Python, describing the hybrid atomic orbitals and the main hydrogen atom parts.

Methodology



1. Cartesian coordinates are defined and converted to spherical coordinates to handle the equations associated with the atom
2. Gouting the cat, the function `<radial function>` is used to calculate the atom radio with the help of the quantum numbers $\boldsymbol{n}$ and $\boldsymbol{l}$.
3. The function `<Spherical>` is required to calculate the orbital's shape and needs the quantum numbers $\boldsymbol{l}$ and $\boldsymbol{m}$.
4. To calculate the probability density function, the quantum numbers $(\boldsymbol{n}, \boldsymbol{l}, \boldsymbol{m})$ are needed and it is written by the next expression $|\psi(n,l,m)|^2$
5. The following linear combinations are calculated $sp\ , sp^2, sp^3, sp^2d, sp^3d\ y\ sp^3d^2$
6. The calculations are represented by plots with the library plotly from python



1. Coordinates

The Schrödinger's equation solution turns too complicated to solve with cartesian coordinates. So, the spherical coordinates are more helpful to solve the equation and represents better the atom's behavior

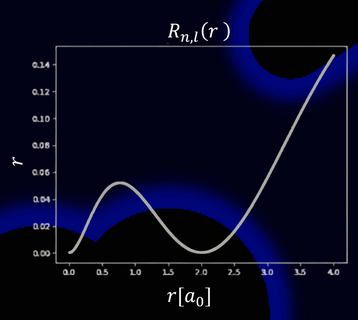
$\boldsymbol{n}$: Energy level.

$\boldsymbol{l}$: Suborbital

$\boldsymbol{m}$: Orbital orientation

2. Quantum Numbers

To solve the Schrödiner's equation, the quantum numbers are calculated. Each number describes the electron's behavior, such as its energy level, suborbital, orbital orientation or the electron's spin ($\boldsymbol{n}$, $\boldsymbol{l}$, $\boldsymbol{m}$ y $\boldsymbol{s}$,). In this work, the three first numbers will be used

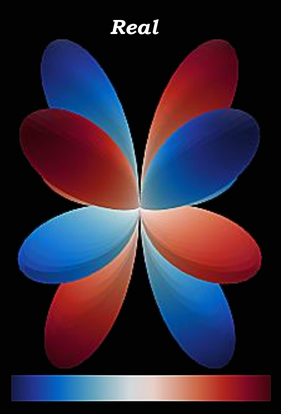


3. Radial Function

The Laguerre's equation is calculated, and uses the quantum numbers $\boldsymbol{n}$ (Orbital level), $\boldsymbol{l}$ (suborbital) and the spherical coordinate $\boldsymbol{\rho}$ as the input. $\boldsymbol{\rho}$ represents a generic space, and the function returns $\boldsymbol{\rho}$ transformed according the quantum numbers $\boldsymbol{n}$ and $\boldsymbol{l}$ and describes the radio between the electron and atom.

$\boldsymbol{n, l, \rho}$

$$R_{nl}(\boldsymbol{\rho}) = \sqrt{\left(\frac{2}{na_0}\right)^3 * \frac{(n-l-1)!}{2n(n+l)!}} e^{-\frac{\rho}{na_0}} \left(\frac{2\boldsymbol{\rho}}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2\boldsymbol{\rho}}{na_0}\right)$$

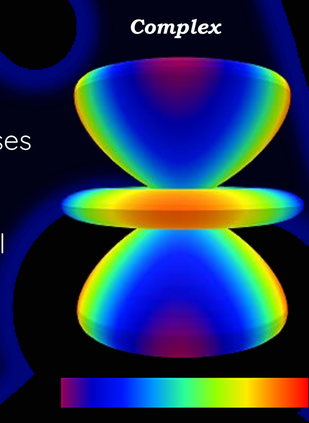


4. Spherical Harmonics Real and complex

The Legendre's equation is calculated and describes the electron's morphology. Which uses the quantum numbers $\boldsymbol{l}$ (suborbital) and $\boldsymbol{m}$ (Orbital orientation). Besides the spherical coordinates θ y ϕ. The function contains a real and an imaginary componets.

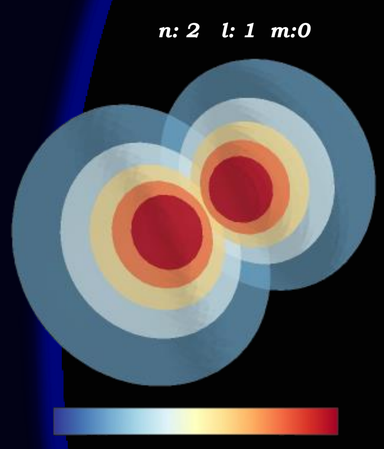
$\boldsymbol{l, m, \theta, \phi}$

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} * \frac{(l-m)!}{(l+m)!}} P_l^m(cos\theta) e^{im\phi}$$



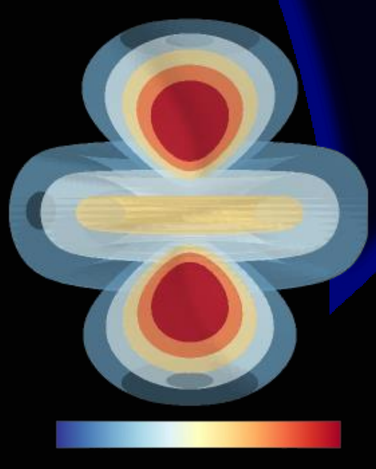
5. Wave Function $\psi_1(n,l,m)$

$\boldsymbol{\rho, \theta, \phi}$



Wave Function $\psi_2(n,l,m)$

$\boldsymbol{\rho, \theta, \phi}$



When the radial and spherical harmonics are joined. It follows the next equation.

$$|\psi(\rho,\theta,\phi)|^2 = |\mathrm{R(r)} * \mathrm{Y}(\theta,\phi)|^2$$

Describing the electron's space inside the atom. This expresión takes the results gotten with the radial and spherical parts, and returns three coordinates represented according with the three quantum numbers n, l, m

The región's probability of the wave function must be 1, that it means, the electron can be found anywhere insde the region.

6. Hybridization

The hybridization is the linear combinations from several vectorial functions denoted with $(\vec{\psi})$ and constants represented with c. The following expresión represents it

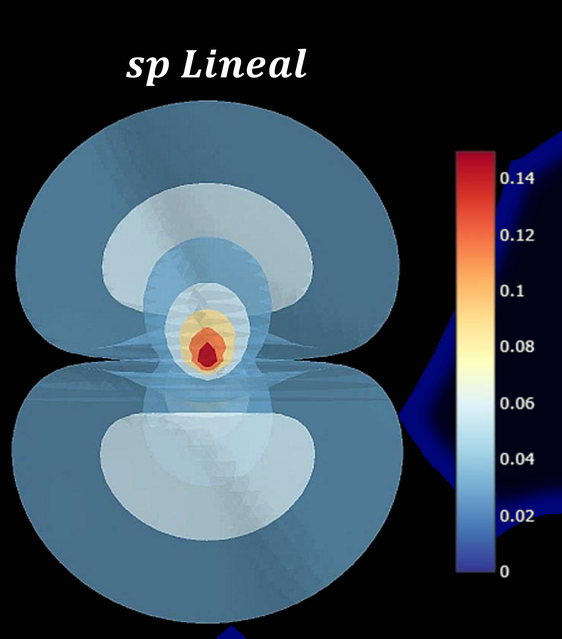
$$(\Psi = c_1\psi_1 + c_2\psi_2 + \cdots + c_n\psi_n).$$

To combine different atoms that are represented as $(\vec{\psi})$. The vectorial functions must be normalized (the functions must have a probability of 1 to be found its electron) and ortogonal (each function must have an inclination of 90 degrees). In the figure, these probabilities are represented with the heat-bar. While the colour is warmer, has more probability to be found.

An example of use for hybridization in chemistry is the covalent bounds

The following linear combinations represents each hybridization lobe:
sp Lineal :

$$Y_{sp}(1) = \frac{1}{\sqrt{2}}\psi_s + \frac{1}{\sqrt{2}}\psi_{p_x}$$
$$Y_{sp}(2) = \frac{1}{\sqrt{2}}\psi_s - \frac{1}{\sqrt{2}}\psi_{p_x}$$



Conclusions:

Despite that the atom structures reviewed in this poster are widely studied, there was not a pedagogical tool to teach these basic structures. The students can find these tool as an introduction to Python and quantum mechanic because the commands are descripted with the parameters reviewed and name functions that are easy to learn

References

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