Classical and Quantum Visualizations of the Hydrogen Atom: Modeling of States, Orbitals, Superpositions, and Quantum Beating

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Abstract

This document describes a three–stage visualization of the hydrogen atom and a simple quantum two–level model based on hydrogenic 1s and 2p wavefunctions. The first visualization shows the stationary orbitals 1s, 2s, 2p$_x$, 2p$_y$, 2p$_z$ and a combined "All" pseudostate. The second visualization illustrates a spatial superposition of 1s and 2p$_z$ in a two–dimensional slice, controlled by real amplitudes and a relative phase. The third visualization depicts time–dependent quantum beating arising from the interference between 1s and 2p$_z$. We compute the physical beating frequency for the hydrogen 1s–2p transition and discuss the predictive character of these results and their relation to experimentally observed ultrafast phenomena.

1 Hydrogenic orbitals and coordinate conventions

We consider the nonrelativistic hydrogen atom in the central Coulomb field of a proton with charge $+e$. The electron has charge $-e$ and mass m_e. The Hamiltonian (in SI units) is

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}, \tag{1}$$

where $r = |\mathbf{r}|$ is the distance from the proton. The stationary states are obtained from the time–independent Schroedinger equation

$$\hat{H}\psi_{nlm}(\mathbf{r}) = E_n\psi_{nlm}(\mathbf{r}), \tag{2}$$

with the well–known hydrogenic energy spectrum

$$E_n = -\frac{13.6\ \text{eV}}{n^2}, \qquad n = 1, 2, 3, \dots \tag{3}$$

In this work we adopt Bohr radius units $a_0 = 1$ for spatial coordinates and consider the hydrogenic wavefunctions in their standard normalized forms. We use Cartesian coordinates (x, y, z) for visualization, but the analytic expressions are more naturally given in spherical coordinates (r, θ, ϕ), with

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta. \tag{4}$$

We focus on the $n = 1$ and $n = 2$ orbitals:

- 1s: $n = 1, l = 0, m = 0$,
- 2s: $n = 2, l = 0, m = 0$,
- 2p: $n = 2, l = 1, m = 0, \pm 1$.

For visualization we use real combinations corresponding to "2p$_x$", "2p$_y$" and the standard "2p$_z$".

2 Analytic forms of the orbitals used in the visualizations

In units $a_0 = 1$ and $Z = 1$ (hydrogen, not just hydrogenic ions), the normalized 1s and 2s orbitals in Cartesian coordinates are:

2.1 1s orbital

The 1s orbital does not depend on the angles:

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi}} e^{-r}. \tag{5}$$

In Cartesian form we write

$$r = \sqrt{x^2 + y^2 + z^2}, \qquad \psi_{1s}(x, y, z) = \frac{1}{\sqrt{\pi}} e^{-r}. \tag{6}$$

The corresponding probability density is

$$|\psi_{1s}|^2 = \frac{1}{\pi} e^{-2r}. \tag{7}$$

2.2 2s orbital

The hydrogenic 2s wavefunction is

$$\psi_{2s}(r) = \frac{1}{4\sqrt{2\pi}} (2 - r) e^{-r/2}, \tag{8}$$

hence

$$\psi_{2s}(x, y, z) = \frac{1}{4\sqrt{2\pi}} \left(2 - \sqrt{x^2 + y^2 + z^2}\right) \exp\left(-\frac{1}{2}\sqrt{x^2 + y^2 + z^2}\right). \tag{9}$$

This orbital has a radial node at $r = 2a_0$, which in our $a_0 = 1$ units corresponds to $r = 2$.

2.3 2p orbitals: 2p$_z$, 2p$_x$, 2p$_y$

The standard $2p_z$ orbital in spherical coordinates is

$$\psi_{2p_z}(r, \theta, \phi) = \psi_{210}(r, \theta, \phi) = \frac{1}{4\sqrt{2\pi}} r e^{-r/2} \cos\theta. \tag{10}$$

Using $\cos\theta = z/r$, we obtain the Cartesian form

$$\psi_{2p_z}(x,y,z) = \frac{1}{4\sqrt{2\pi}} z e^{-r/2}, \qquad r = \sqrt{x^2+y^2+z^2}. \tag{11}$$

Similarly, by cyclic rotation of axes, we define

$$\psi_{2p_x}(x,y,z) = \frac{1}{4\sqrt{2\pi}} x e^{-r/2}, \qquad \psi_{2p_y}(x,y,z) = \frac{1}{4\sqrt{2\pi}} y e^{-r/2}. \tag{12}$$

These are commonly used real combinations of the $2p_m$ spherical harmonics and correspond to dumbbell–shaped orbitals oriented along the x, y and z axes.

3 Visualization 1: 3D clouds of orbitals and the "All" pseudostate

3.1 Sampling method for point clouds

In the first visualization we show point clouds distributed according to the probability density $|\psi_{nlm}|^2$ for each orbital. For a given orbital $\psi(\mathbf{r})$, we want to draw N points $\mathbf{r}_k$ with

$$P(\mathbf{r}) \propto |\psi(\mathbf{r})|^2. \tag{13}$$

We implement rejection sampling in a bounding cube $[-R_{\text{max}}, R_{\text{max}}]^3$:

1. Precompute $p_{\text{max}} \approx \max_{\mathbf{r}} |\psi(\mathbf{r})|^2$ on a coarse grid.
2. Repeat until N points are accepted:
    (a) Propose (x,y,z) uniformly in the cube.
    (b) Compute $p = |\psi(x,y,z)|^2$.
    (c) Draw u uniformly in $[0, p_{\text{max}}]$.
    (d) If $u < p$, accept the point.

This gives us a point cloud that visually represents the stationary probability distribution for that orbital.

3.2 Individual orbitals

For each of the five orbitals 1s, 2s, 2p$_x$, 2p$_y$, 2p$_z$:

- **1s**: cloud roughly spherical, high density near the proton and falling off as e^{-2r}.
- **2s**: cloud with an inner lobe and outer shell, with a radial node near $r = 2$. We use two colors (inner and outer) to emphasize the node.
- **2p$_x$**: dumbbell–like cloud along the x axis, with a nodal plane at $x = 0$.
- **2p$_y$**: dumbbell–like cloud along the y axis, with a nodal plane at $y = 0$.
- **2p$_z$**: dumbbell–like cloud along the z axis, with a nodal plane at $z = 0$.

The proton is shown as a bright point at the origin $(0,0,0)$. A button–based UI toggles between orbitals so that each cloud can be inspected separately.

3.3 The “All” pseudostate

The “All” mode is not a true eigenstate of the Hamiltonian, and it is not meant to represent the actual ground state of hydrogen (which has only one electron). Rather, it is a visual pseudostate in which all five orbital point clouds are displayed simultaneously:

$$\text{“All”} \quad \Longleftrightarrow \quad \psi_{1s},\ \psi_{2s},\ \psi_{2p_x},\ \psi_{2p_y},\ \psi_{2p_z} \text{ all visible.} \tag{14}$$

This gives an intuitive picture of how different stationary states occupy and structure the spatial region around the proton.

4 Visualization 2: 2D reference 2p$_z$ and static 1s+2p$_z$ superposition

4.1 Two–state superposition ansatz

We now restrict the Hilbert space to a two–dimensional subspace spanned by $\{\psi_{1s}, \psi_{2p_z}\}$. Any state in this subspace can be written as

$$\psi_{\text{tot}}(\mathbf{r}) = A_1\psi_{1s}(\mathbf{r}) + A_2\psi_{2p_z}(\mathbf{r})e^{i\varphi}, \tag{15}$$

where A_1 and A_2 are (generally complex) amplitudes and φ is the relative phase. In our visualization we:

- take A_1 and A_2 to be real, nonnegative sliders,
- put the entire phase difference into the factor $e^{i\varphi}$.

In a fully normalized quantum state, one would impose

$$\int |\psi_{\text{tot}}(\mathbf{r})|^2 d^3r = 1, \tag{16}$$

which constrains A_1 and A_2. During interactive visualization we do not enforce this normalization at every slider update; instead, we rescale the resulting density to the colormap range.

4.2 Physical interpretation of A_1, A_2, φ

The coefficients A_1 and A_2 are dimensionless expansion coefficients. If the state

$$|\psi\rangle = A_1|1s\rangle + A_2e^{i\varphi}|2p_z\rangle \tag{17}$$

were normalized so that $|A_1|^2 + |A_2|^2 = 1$, then $|A_1|^2$ and $|A_2|^2$ would be the probabilities of finding the electron in the 1s or 2p$_z$ eigenstates upon an energy measurement.

The phase φ is a relative phase between the two components. It has no direct classical geometric analog, but it enters the interference term in the probability density:

$$|\psi_{\text{tot}}|^2 = |A_1|^2|\psi_{1s}|^2 + |A_2|^2|\psi_{2p_z}|^2 + 2\Re\left(A_1A_2^*\psi_{1s}\psi_{2p_z}^*e^{i\varphi}\right). \tag{18}$$

Changing φ shifts how constructive or destructive interference occurs in different spatial regions, thereby redistributing the probability density $|\psi_{\text{tot}}|^2$ even though the total probability remains unity after normalization.

4.3 2D slice and reference 2p$_z$

For visualization we again restrict to the $y = 0$ plane. On a 2D grid

$$x \in [-R_{\max}, R_{\max}], \quad z \in [-R_{\max}, R_{\max}], \tag{19}$$

we define

$$\psi_{1s}^{(2D)}(x,z) = \psi_{1s}(x,0,z), \quad \psi_{2p_z}^{(2D)}(x,z) = \psi_{2p_z}(x,0,z). \tag{20}$$

The total wavefunction in this slice is

$$\psi_{\text{tot}}^{(2D)}(x,z) = A_1\psi_{1s}^{(2D)}(x,z) + A_2\psi_{2p_z}^{(2D)}(x,z)e^{i\varphi}. \tag{21}$$

The second visualization now consists of two panels:

- Left panel: the reference density

  $$|\psi_{2p_z}^{(2D)}(x,z)|^2 = |\psi_{2p_z}(x,0,z)|^2, \tag{22}$$

  which clearly shows the dumbbell–like structure (two lobes in the $z > 0$ and $z < 0$ regions) and the node at $z = 0$.

- Right panel: the superposition density

  $$|\psi_{\text{tot}}^{(2D)}(x,z)|^2, \tag{23}$$

  which responds to changes of A_1, A_2, and φ via the interference term in (**??**).

By adjusting the sliders for A_1, A_2, and φ, one can see how the spatial pattern shifts from approximately 1s–like to approximately 2p$_z$–like and how the relative phase φ moves probability density between the upper and lower lobes.

5 Visualization 3: quantum beating between 1s and 2p$_z$

5.1 Time–dependent two–level superposition

In the full time–dependent description, the stationary states evolve as

$$\psi_{1s}(\mathbf{r},t) = \psi_{1s}(\mathbf{r})e^{-iE_1t/\hbar}, \quad \psi_{2p_z}(\mathbf{r},t) = \psi_{2p_z}(\mathbf{r})e^{-iE_2t/\hbar}. \tag{24}$$

A general two–state superposition is

$$\psi(\mathbf{r},t) = c_1\psi_{1s}(\mathbf{r})e^{-iE_1t/\hbar} + c_2\psi_{2p_z}(\mathbf{r})e^{-iE_2t/\hbar}. \tag{25}$$

Factoring out a global phase $e^{-iE_1t/\hbar}$ that does not affect probabilities, one finds

$$\psi(\mathbf{r},t) = e^{-iE_1t/\hbar}\left[c_1\psi_{1s}(\mathbf{r}) + c_2\psi_{2p_z}(\mathbf{r})e^{-i(E_2-E_1)t/\hbar}\right]. \tag{26}$$

The relative phase between the 1s and 2p$_z$ components is therefore

$$\varphi(t) = \frac{(E_2 - E_1)t}{\hbar} = \omega t, \tag{27}$$

where

$$\omega = \frac{|E_2 - E_1|}{\hbar} \tag{28}$$

is the physical angular frequency of the 1s–2p quantum beating.

5.2 Physical beating frequency for the hydrogen 1s–2p transition

The hydrogenic energy levels (ignoring fine structure) are

$$E_n = -\frac{13.6\ \text{eV}}{n^2}. \tag{29}$$

Hence:

$$E_1 = -13.6\ \text{eV}, \qquad E_2 = -\frac{13.6}{4} \approx -3.4\ \text{eV}. \tag{30}$$

The energy difference is

$$\Delta E = E_2 - E_1 \approx -3.4 - (-13.6) = 10.2\ \text{eV}. \tag{31}$$

We convert this to joules using

$$1\ \text{eV} \approx 1.602 \times 10^{-19}\ \text{J}, \tag{32}$$

so

$$|\Delta E| \approx 10.2 \times 1.602 \times 10^{-19} \approx 1.63 \times 10^{-18}\ \text{J}. \tag{33}$$

The reduced Planck constant is

$$\hbar \approx 1.055 \times 10^{-34}\ \text{J s}. \tag{34}$$

Therefore, the physical angular frequency of 1s–2p beating is

$$\omega_{\text{phys}} = \frac{|\Delta E|}{\hbar} \approx \frac{1.63 \times 10^{-18}}{1.055 \times 10^{-34}} \approx 1.5 \times 10^{16}\ \text{s}^{-1}. \tag{35}$$

The corresponding period is

$$T_{\text{phys}} = \frac{2\pi}{\omega_{\text{phys}}} \approx \frac{6.283}{1.5 \times 10^{16}} \approx 4 \times 10^{-16}\ \text{s}. \tag{36}$$

Thus, an ideal coherent superposition of 1s and 2p$_z$ in hydrogen would exhibit oscillations in $|\psi(\mathbf{r}, t)|^2$ with a period on the order of 4×10^{-16} s (a few tenths of a femtosecond). Because the $2p$ state has a finite lifetime (of order 10^{-9} s), in principle many millions of such oscillations could occur before radiative decay, although the actual behavior in a realistic environment is complicated by spontaneous emission and decoherence.

5.3 Beating visualization and rescaled time

In our third visualization we simulate these quantum beatings in the 2D plane $y = 0$ as

$$\psi^{(2D)}(x, z, t) = A_1 \psi_{1s}^{(2D)}(x, z) + A_2 \psi_{2p_z}^{(2D)}(x, z) e^{i\varphi(t)}, \quad \varphi(t) = \omega_{\text{vis}} t, \tag{37}$$

where A_1 and A_2 are chosen (for example) as $A_1 = 0.5$ and $A_2 = 2.0$ to emphasize the 2p$_z$ structure, and ω_{vis} is a *visual* angular frequency chosen for perceptual clarity (rather than equal to ω_{phys}). For each time step t_k we compute

$$\psi^{(2D)}(x, z, t_k) = A_1 \psi_{1s}^{(2D)}(x, z) + A_2 \psi_{2p_z}^{(2D)}(x, z) e^{i\omega_{\text{vis}} t_k} \tag{38}$$

and display the corresponding density $|\psi^{(2D)}(x, z, t_k)|^2$ as a color map.

We note that:

- The *spatial* structure in all three visualizations is based on exact analytic hydrogenic orbitals (1s, 2s, 2p$_x$, 2p$_y$, 2p$_z$).
- The *temporal* dependence in Visualization 3 is scaled and slowed down relative to the physical timescale $T_{\text{phys}} \sim 4 \times 10^{-16}$ s, so that the beating pattern can be seen evolving by eye.

6 Summary and predictive character of the model

We have presented a three–stage visualization framework for the hydrogen atom:

1. **Visualization 1:** 3D point–cloud representations of individual hydrogenic orbitals 1s, 2s, $2p_x$, $2p_y$, $2p_z$ and a combined "All" pseudostate. This shows the spatial forms, nodes, and orientations of the standard hydrogenic eigenfunctions.
2. **Visualization 2:** A 2D slice ($y = 0$) showing, on the left, the pure $2p_z$ density $|\psi_{2p_z}(x, 0, z)|^2$ and, on the right, the superposition density $|\psi_{\mathrm{tot}}(x, 0, z)|^2$ for $\psi_{\mathrm{tot}} = A_1\psi_{1s} + A_2\psi_{2p_z}e^{i\varphi}$. Amplitudes A_1, A_2, and the phase φ are controlled by sliders, revealing how interference reshapes $|\psi|^2$.
3. **Visualization 3:** A time–dependent 2D pattern illustrating quantum beating between 1s and $2p_z$. The left panel shows the static pure $2p_z$ reference, while the right panel depicts the evolving superposition density $|\psi(x, 0, z, t)|^2$ driven by a relative phase $\varphi(t) = \omega t$. The physical beating frequency for the 1s–2p hydrogenic transition is $\omega_{\mathrm{phys}} \approx 1.5 \times 10^{16}\ \mathrm{s}^{-1}$ (period $T_{\mathrm{phys}} \approx 4 \times 10^{-16}$ s), while the visualization employs a rescaled ω_{vis} for clarity.

The spatial part of our model is strictly based on the exact analytic solutions of the nonrelativistic hydrogenic Schroedinger equation. Within the two–level subspace $\{1s, 2p_z\}$, the structure of the superposition and the quantum beating frequency follow directly and rigorously from standard quantum mechanics.

At the same time, the predictions regarding the detailed spatial time–evolution of the 1s–$2p_z$ superposition at the attosecond to femtosecond timescale remain largely *predictive* in character: they are inferred from the theory but, due to the extremely high frequencies and short periods involved, cannot be directly imaged as real–space density movies with present experimental techniques.

However, these theoretical predictions are *consistent* with and supported by a variety of experimental observations in ultrafast and strong–field physics, including:

- time–resolved pump–probe measurements of excited–state populations and coherences in atomic hydrogen and hydrogen–like ions;
- attosecond transient absorption spectroscopy, in which oscillatory modulations of absorption lines reflect coherent superpositions of bound states with energy differences on the order of tens of eV;
- Rydberg–wave–packet experiments, where quantum beating between closely spaced high–n hydrogenic states has been directly observed in time–resolved signals;
- high–harmonic generation and strong–field ionization studies, whose spectra and temporal modulations are sensitive to the phase evolution of bound–state superpositions and continuum wavepackets;
- Ramsey–type interference measurements and quantum beat spectroscopy in atoms and molecules, where oscillatory signals at frequencies $|E_i - E_j|/\hbar$ are experimentally detected.

In this sense, our three–stage modeling and visualization can be regarded as a predictive, theory–driven picture that extrapolates well–validated quantum–mechanical principles into a spatially explicit, time–dependent representation. While the exact real–space density movies of the 1s–2p$_z$ beating are not yet directly measured, the underlying frequency scales and coherence phenomena are in close agreement with experimental evidence from ultrafast spectroscopy, Rydberg dynamics, and strong–field experiments.

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*: Modeling, calculations and material preparation were performed using mshell. Mshell is a minimalistic Unix shell designed for resource-constrained environments, combining traditional shell functionality with integrated AI capabilities through local LLM models via Ollama or Linux LLM evaluation framework (current version of mshell is 1.4.1), cloud LLMs, especially Ollama cloud models, Claude by Anthropic and ChatGPT from OpenAI.