## Visualize a coherence between hydrogenic s and p states

Define grid for angular part of wavefunction

$i := 0 .. 100$

$\theta_i := \frac{i \cdot 2 \cdot \pi}{100}$

set electron density cutoff at which we will plot orbital: $\sigma := 1$

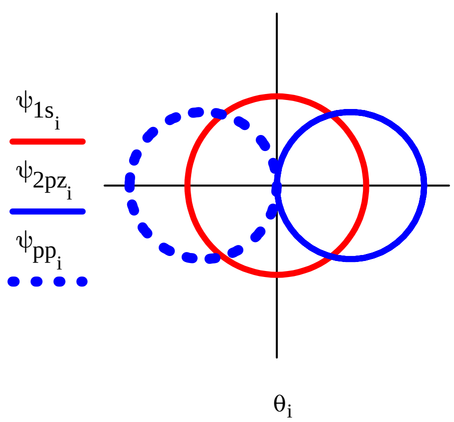
Use 1s and 2pz orbitals

$\psi_{1s_i} := \frac{1}{\sqrt{\pi}} \cdot e^{-\sigma}$ $\psi_{2pz_i} := \frac{\cos(\theta_i)}{\sqrt{\pi}} \cdot \sigma \cdot e^{-\frac{\sigma}{2}}$ $\psi_{pp} := -\psi_{2pz}$

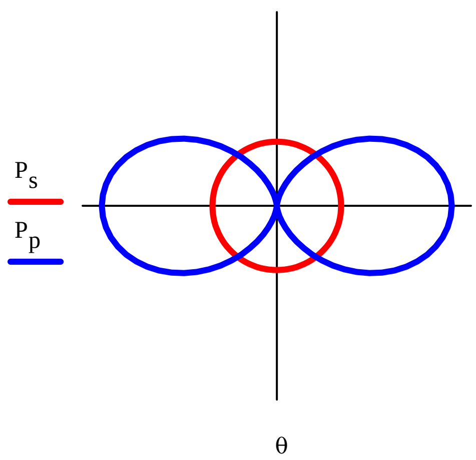
$P_{s_i} := \left(\psi_{1s_i}\right)^2$ Angular dependence of 1s electron density

$P_{p_i} := \left(\psi_{2pz_i}\right)^2$ Angular dependence of $2p_z$ electron density

Basis Wavefunctions




Basis state prob. density



**Visualize a static superposition:**

Set amplitude ( between -1 to 1): $c_s := 0.5$ $c_p := \sqrt{1 - (|c_s|)^2}$ $c_p = 0.866$

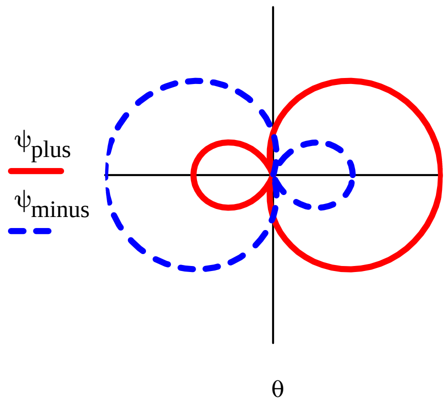
$$\psi_{plus_i} := \left| c_s \cdot \psi_{1s_i} + c_p \cdot \psi_{2pz_i} \right|$$

$$\psi_{minus_i} := \left| c_s \cdot \psi_{1s_i} - c_p \cdot \psi_{2pz_i} \right|$$

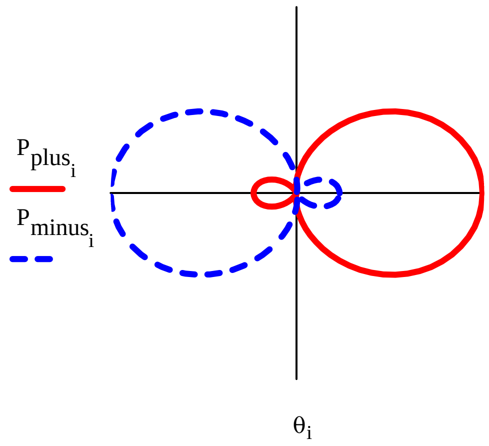
$$P_{plus_i} := \left( c_s \cdot \psi_{1s_i} + c_p \cdot \psi_{2pz_i} \right)^2$$

$$P_{minus_i} := \left( c_s \cdot \psi_{1s_i} - c_p \cdot \psi_{2pz_i} \right)^2$$

Superposition




Probability distribution



## Visualize a Time-Dependent Wavefunction

Frequency splitting: $\Delta := 1$ $\quad V := 1$

Rabi frequency: $\Omega := \sqrt{V^2 + \Delta^2}$ $\quad \Omega = 1.414$

Define a time grid: $j := 0 .. 500$ $\quad \tau_j := \frac{j \cdot \Omega}{2 \cdot \pi \cdot 5}$

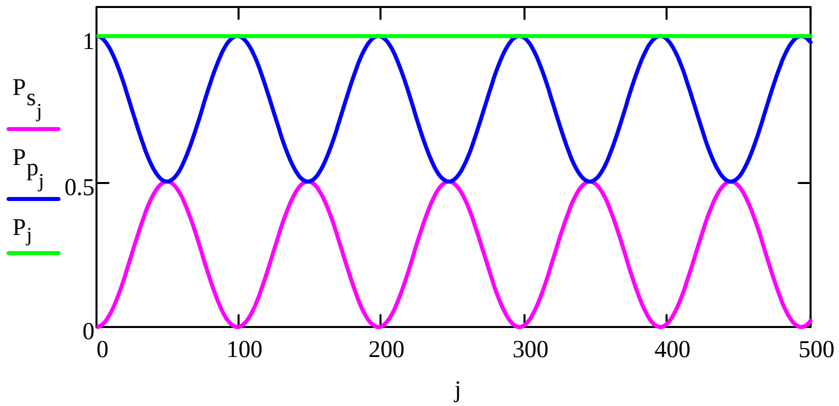
Complex amplitudes:

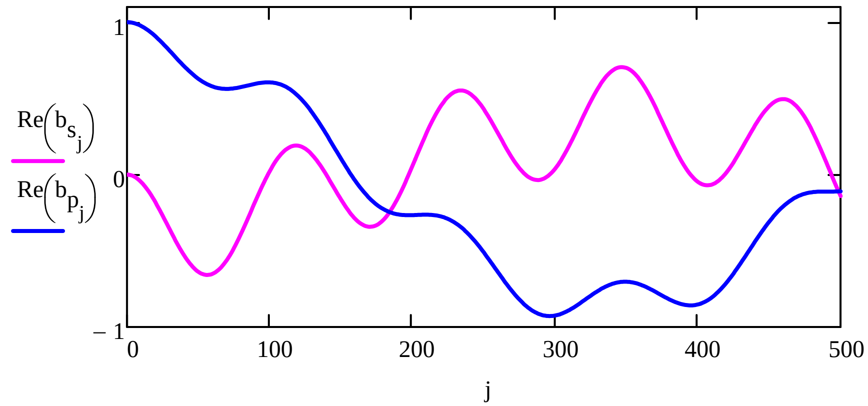
$$b_{s_j} := \frac{-i \cdot V}{\Omega} \cdot e^{-i \cdot \frac{\Delta \cdot \tau_j}{2}} \cdot \sin\left(\frac{\Omega}{2} \cdot \tau_j\right) \qquad b_{p_j} := e^{\frac{i \cdot \Delta \cdot \tau_j}{2}} \cdot \left(\cos\left(\frac{\Omega}{2} \cdot \tau_j\right) - i \cdot \frac{\Delta}{\Omega} \cdot \sin\left(\frac{\Omega}{2} \cdot \tau_j\right)\right)$$

Graph limits: $g := 0.8$

Probability Density

$$P_{s_j} := \left(\left|b_{s_j}\right|\right)^2 \qquad P_{p_j} := \left(\left|b_{p_j}\right|\right)^2 \qquad P := P_s + P_p \qquad \psi_{i,j} := \left|b_{s_j} \cdot \psi 1s_i + b_{p_j} \cdot \psi 2pz_i\right|$$



**Time-Dependent Magnitude of Wavefunction**

Probability density oscillates as one might expect for interaction with a light field.