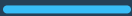


Quantum VR

Andrew Douglas



Outline



1. Rejection Sampling

Stochastic point generation for arbitrary probability densities.



2. Particle in a Box

Probability cloud for a particle in a 3D finite square well.



3. Atomic Orbitals

Probability distribution for electron orbitals.

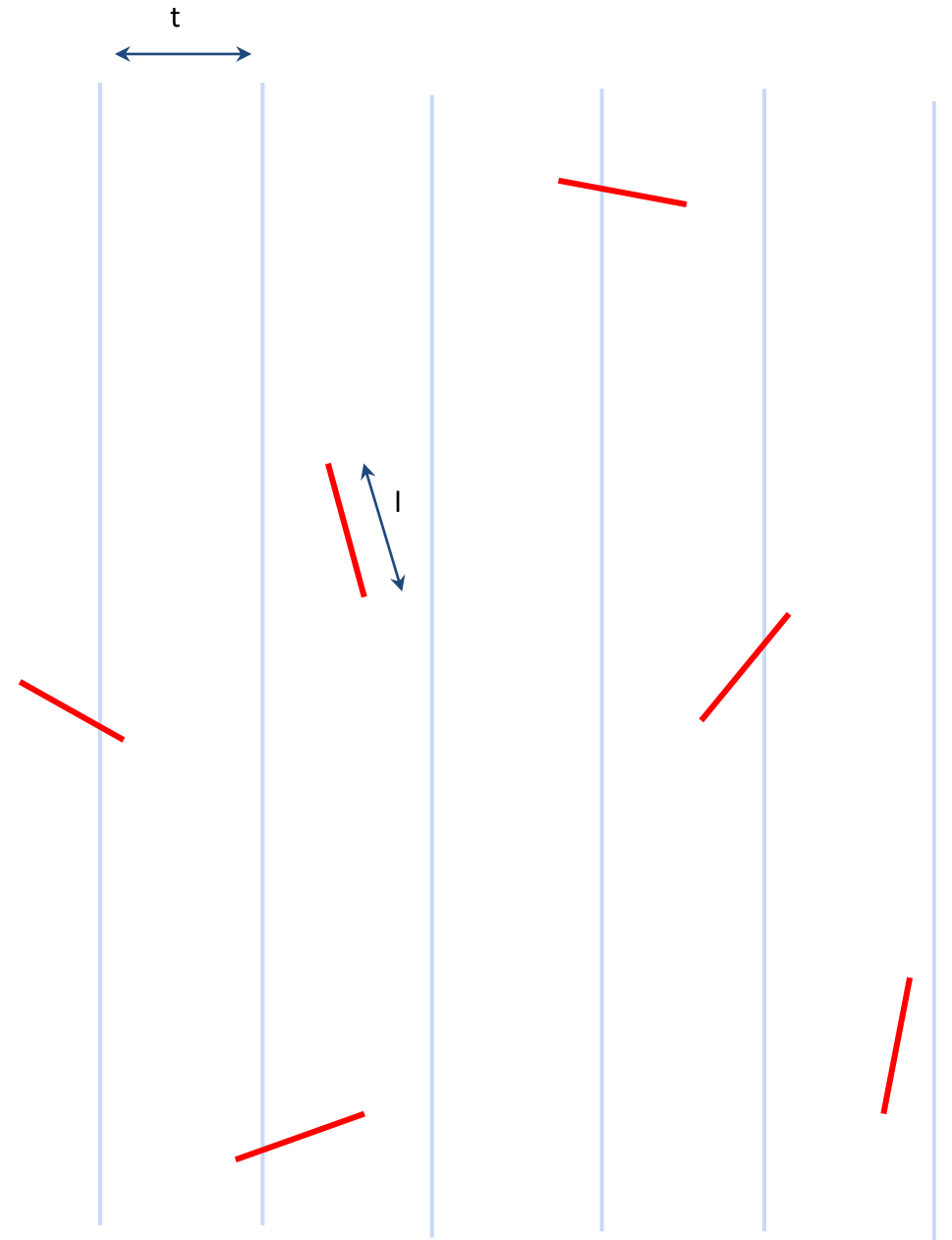
Rejection Sampling

Stochastic point generation for arbitrary probability densities.

Buffon's Needle

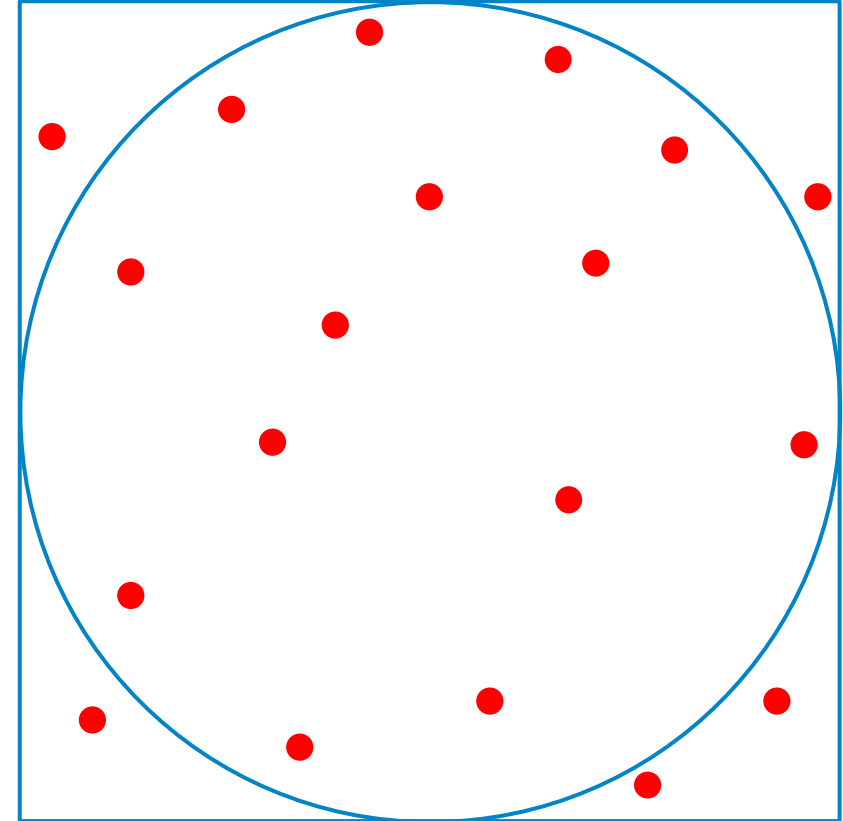
- Suppose you have equally spaced lines of string across the floor
- Drop a needle on this floor
- **What is the probability that a needle intersects a string?**

$$p = \frac{2}{\pi} \cdot \frac{l}{t}$$



Monte Carlo Rejection Sampling

- How do we use this?
- Generate random point in a given bounds
- Roll a target probability
- If $P(\text{random point}) \geq P(\text{target})$, generate a particle at this point
- **How do we find probability function?**

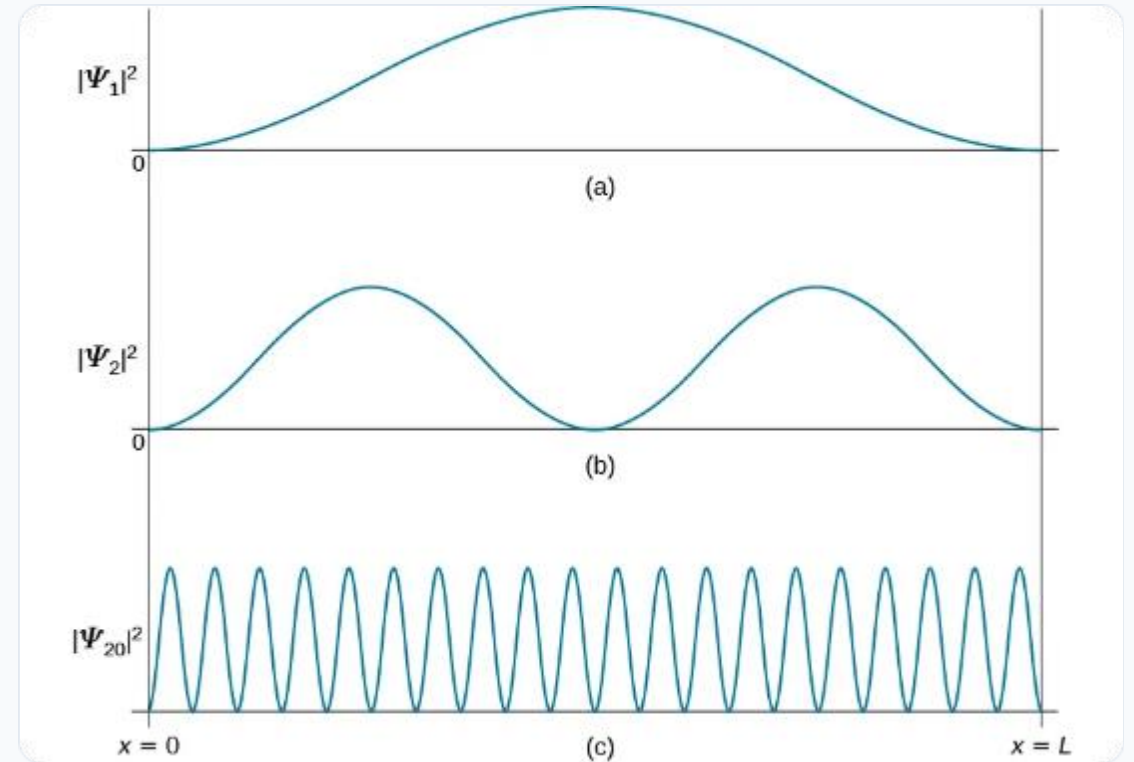


Particle in a Box

Probability cloud for a particle in a 3D finite square well.

What is Particle in a Box?

- A free particle is surrounded by impenetrable barriers ($V = \infty$)
- Particle can only be in certain states, with quantum number n
- Wavefunction takes the form of standing waves with n antinodes
- Square the wavefunction for **probability density**
- Particle can be in ground state ($n=1$), or excited states ($n>1$)
- Likewise, energy can only take certain energy levels. increases with n^2 .



3D Wavefunction, Probability Density, and Energy

Spatial Wavefunction $\Psi(x,y,z)$

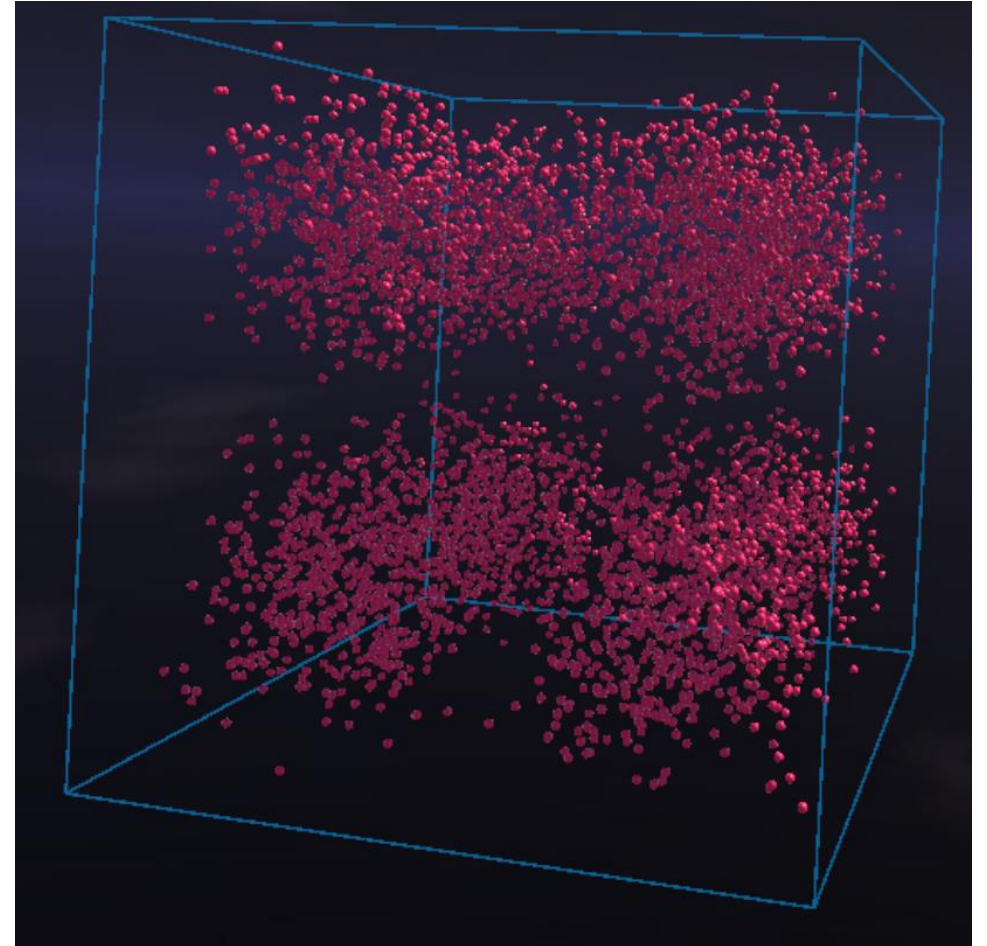
$$\psi_{n_x, n_y, n_z}(x, y, z) = \left(\sqrt{\frac{2}{L}}\right)^3 \sin\left(\frac{n_x \pi x'}{L}\right) \sin\left(\frac{n_y \pi y'}{L}\right) \sin\left(\frac{n_z \pi z'}{L}\right)$$

Probability Density $P(x,y,z)$

$$P(x, y, z) = \frac{8}{L^3} \sin^2\left(\frac{n_x \pi x'}{L}\right) \sin^2\left(\frac{n_y \pi y'}{L}\right) \sin^2\left(\frac{n_z \pi z'}{L}\right)$$

Energy Eigenvalues E

$$E_{n_x, n_y, n_z} = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$

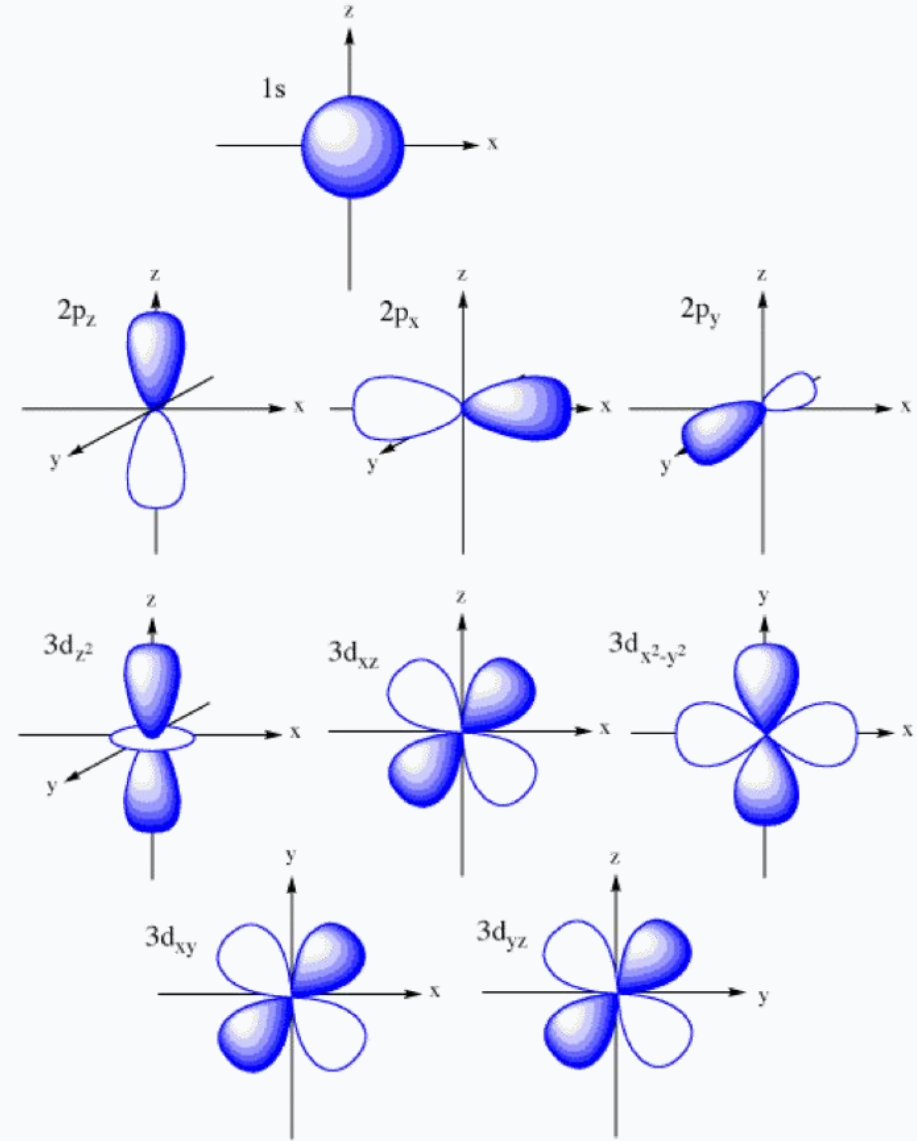
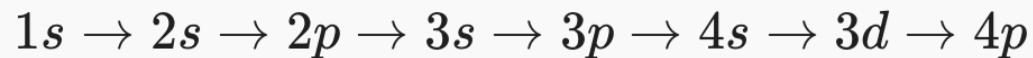


Atomic Orbitals

Probability distribution for electron orbitals.

Atomic Orbitals

- Orbitals are **3D probability clouds**
- Use 3 quantum numbers: n , l , and m
- 4 types of orbitals: s, p, d, and f (determined by l)
- As atom gains electrons, they fill in a specific order
- (Simulation up to $Z = 36$)



Wavefunction, Probability Density, and Energy

Spatial Wavefunction $\Psi(r, \theta, \phi)$

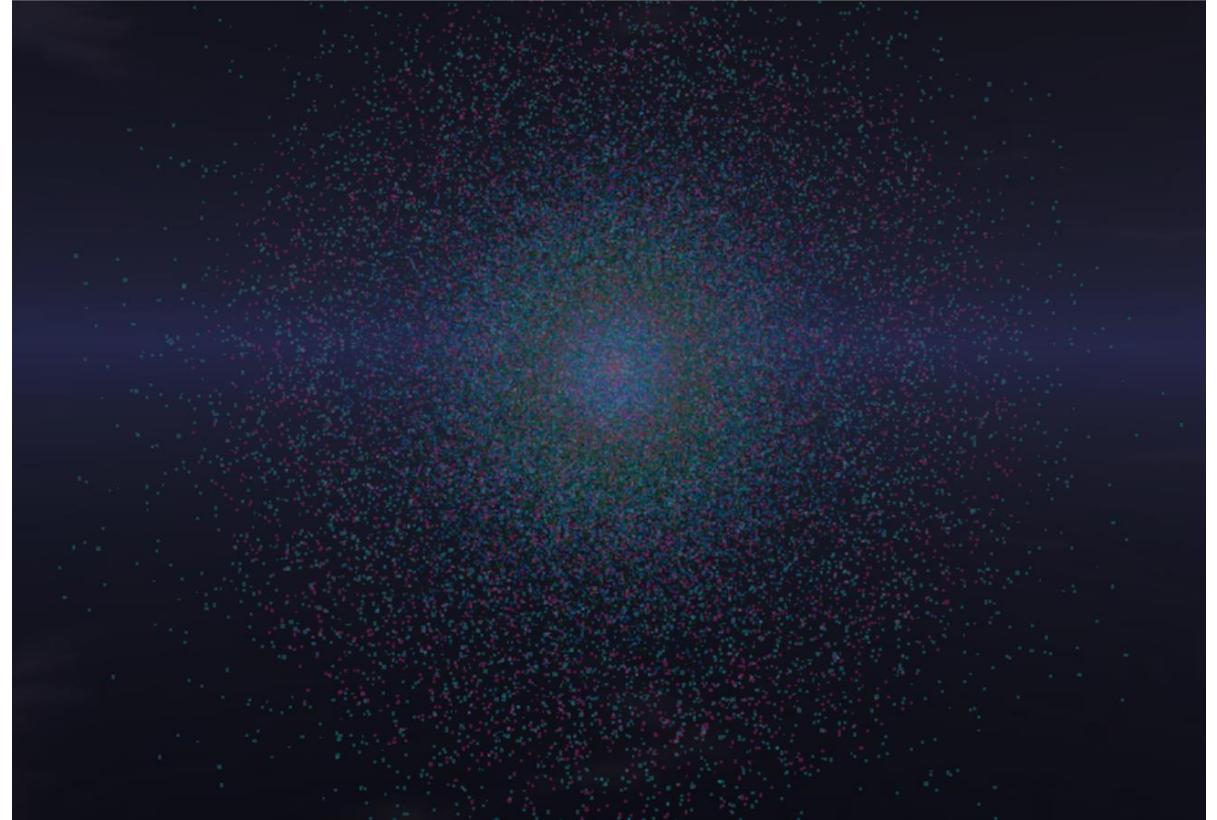
$$\psi_{n,l,m_l}(r, \theta, \phi) = R_{n,l}(r)Y_l^{m_l}(\theta, \phi)$$

Probability Density $P(r, \theta, \phi)$

$$P(r, \theta, \phi) = |\psi_{n,l,m_l}(r, \theta, \phi)|^2 = |R_{n,l}(r)|^2 |Y_l^{m_l}(\theta, \phi)|^2$$

Energy Eigenvalues E

$$E_n = -\frac{\mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{Z^2}{n^2} \approx -13.6 \text{ eV} \cdot \frac{Z^2}{n^2}$$



Questions?

Thank you!