Atomic Structure and Periodicity

Shielding and Such

Shielding

- In a multielectron system, electrons are simultaneously attracted to the nucleus and repelled by each other.
- Outer electrons are *shielded* from the nucleus by the core electrons.
  - ✓Shielding effect
  - ✓Outer electrons do not effectively screen for each other.
- The shielding causes the outer electrons to not experience the full strength of the nuclear charge.

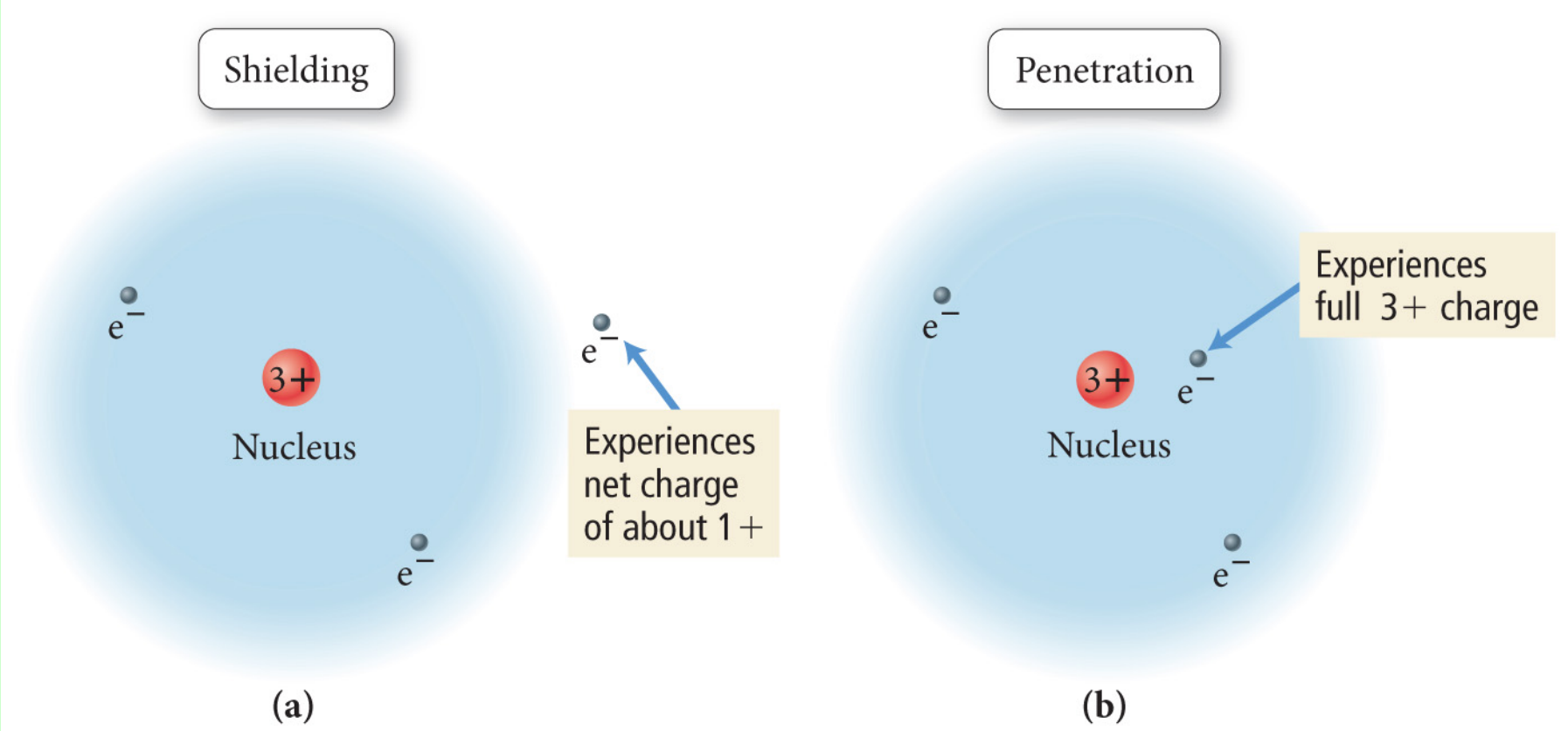
Effective Nuclear Charge

- The **effective nuclear charge** is a net positive charge that is attracting a particular electron.

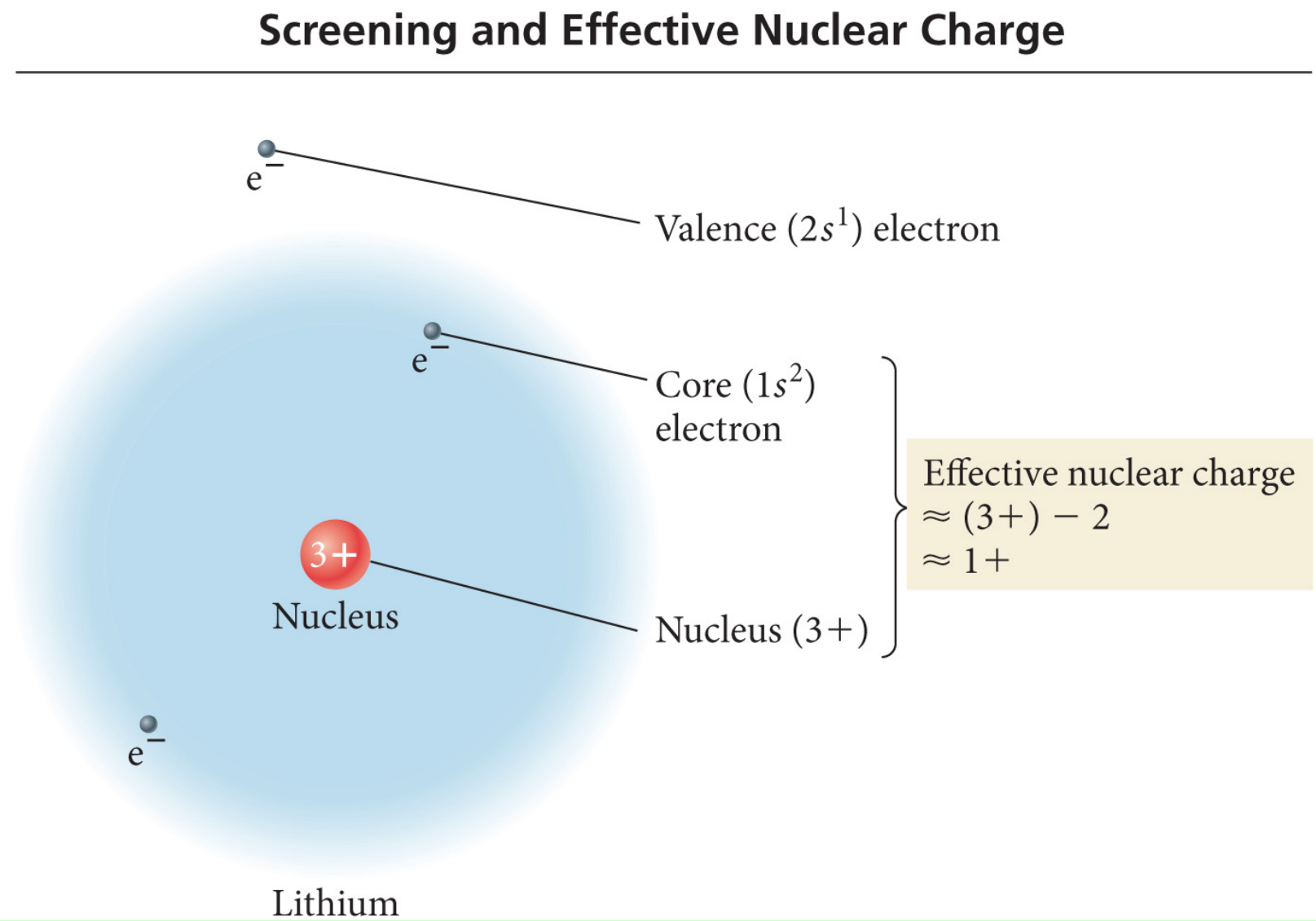
- **Z** is the nuclear charge, and **S** is the number of electrons in lower energy levels.
  - Electrons in the same energy level contribute to screening but since their contribution is so small they are not part of the calculation.
  - Trend is *s* > *p* > *d* > *f*.

$$Z_{effective} = Z - S$$

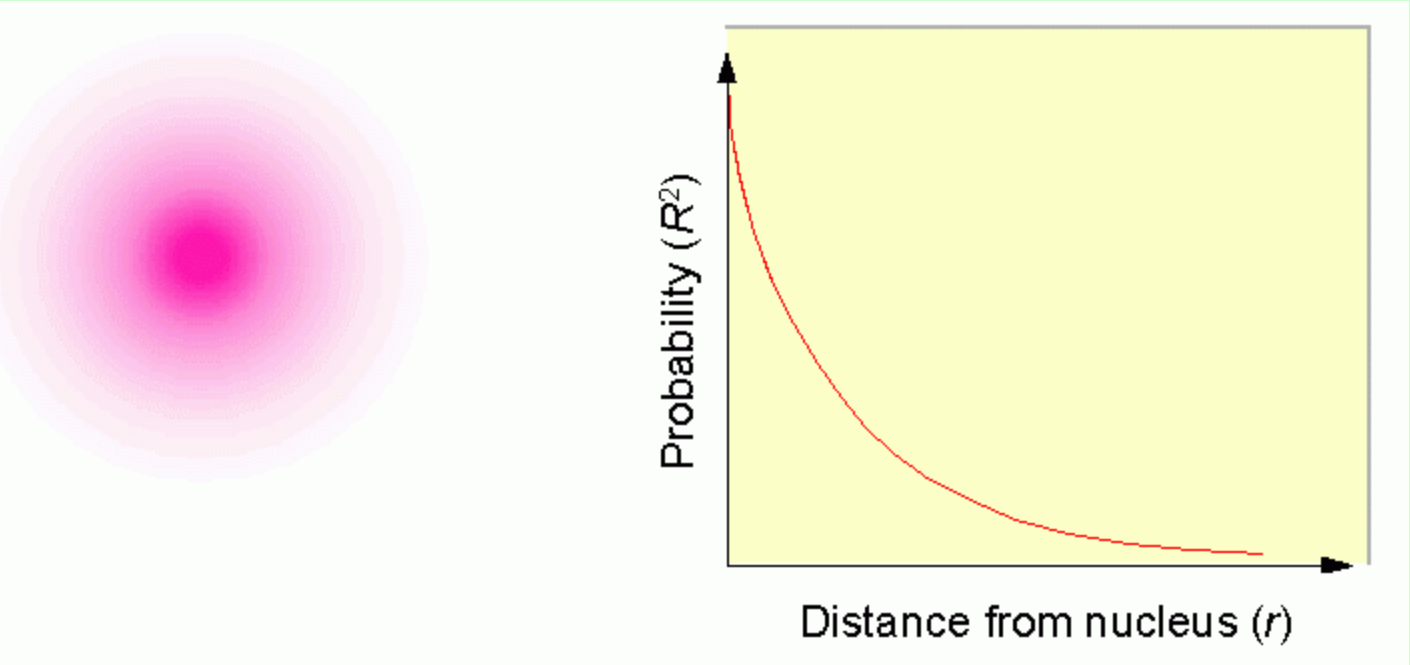
Shielding and Penetration



Shielding and Effective Nuclear Charge



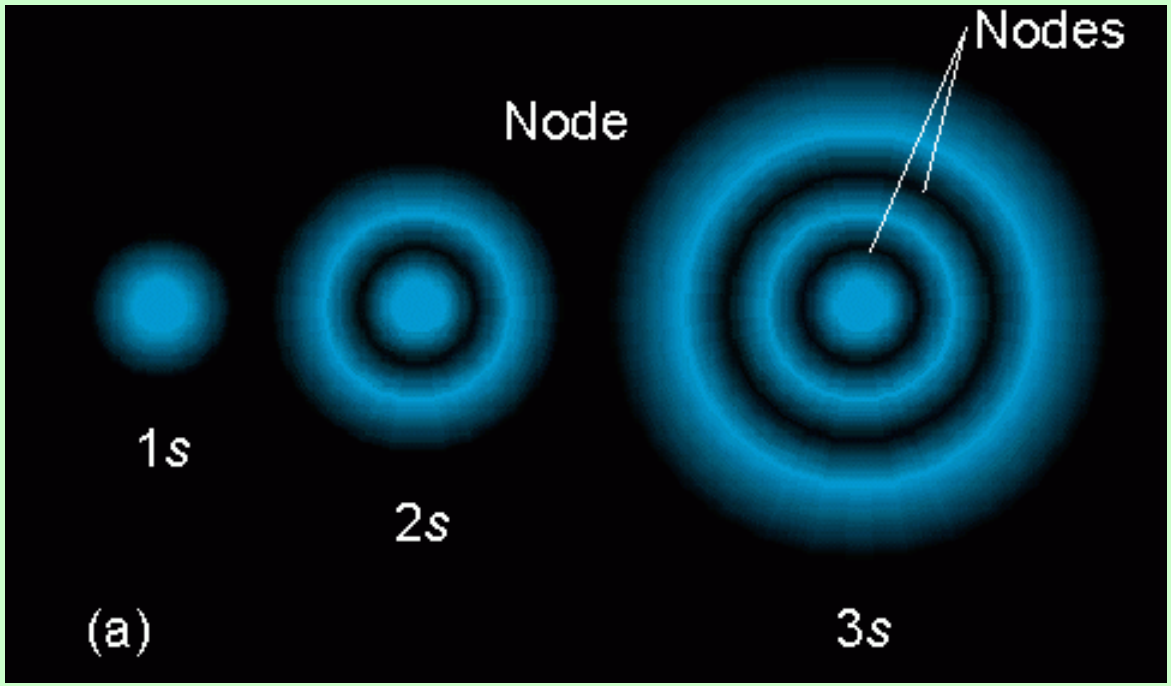
An orbital is a region within an atom where there is a probability of finding an electron. This is a probability diagram for the s orbital in the <u>first energy level…</u>



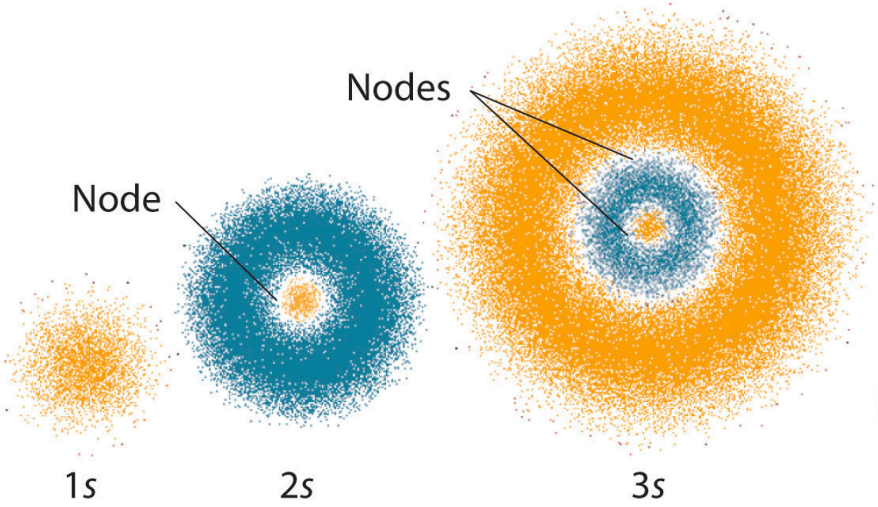
Orbital shapes are defined as the surface that contains 90% of the total electron probability.

Sizes of *s* orbitals

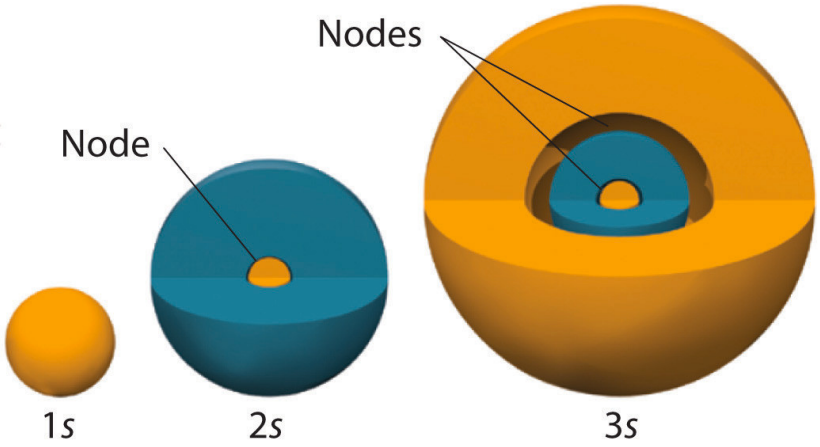
Orbitals of the same shape (s, for instance) grow larger as n increases…



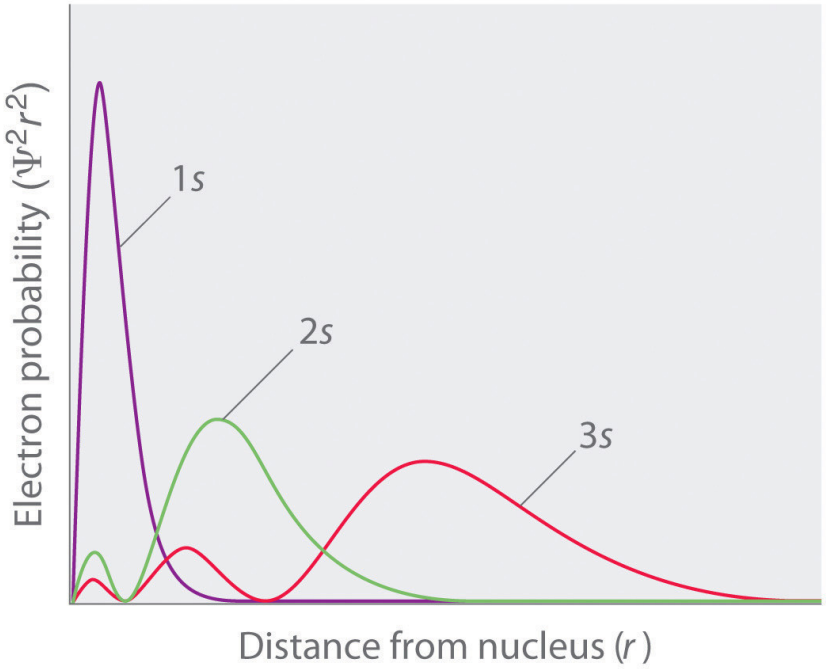
Nodes are regions of low probability within an orbital.



(a) Electron probability



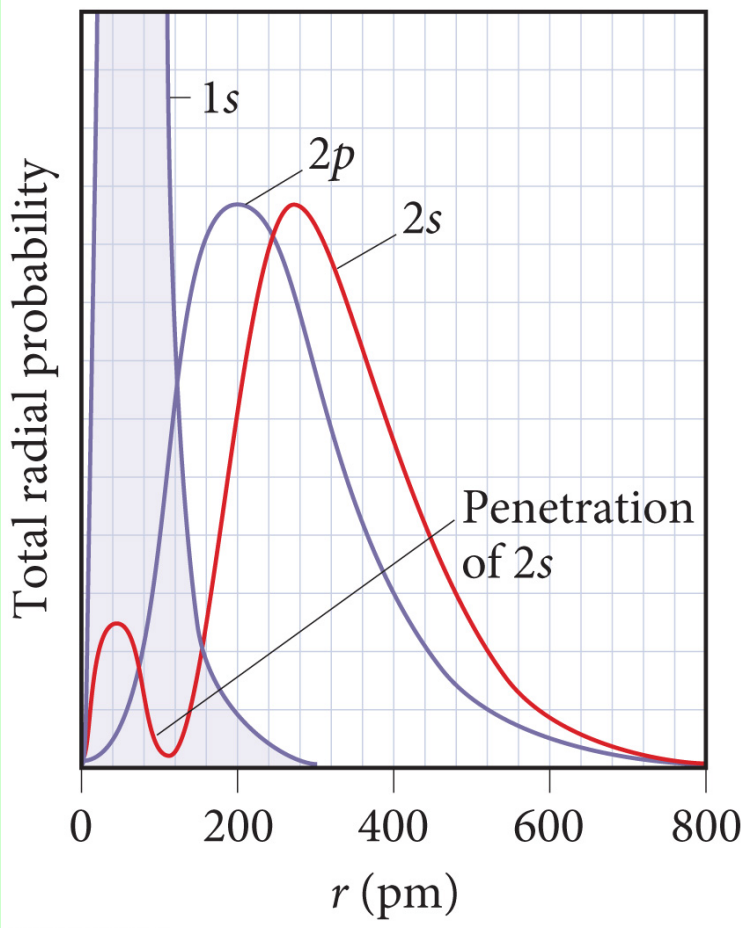
(b) Contour probability



(c) Radial probability

Penetration and Shielding

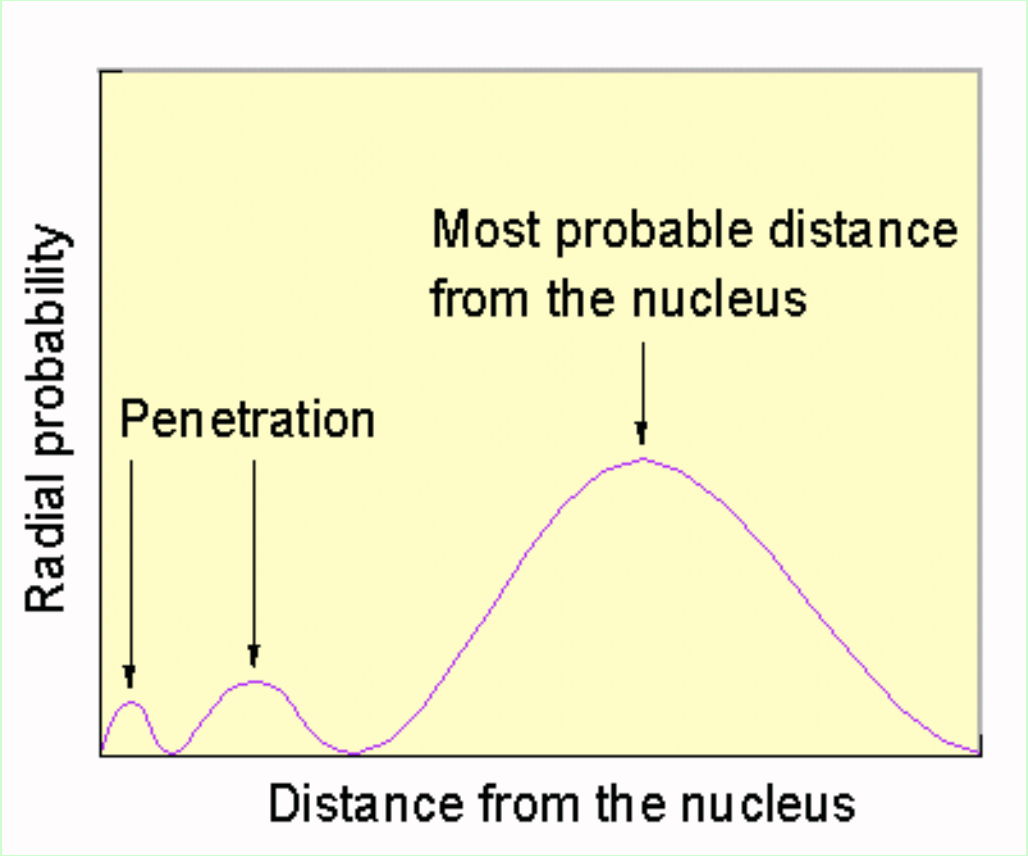
- The radial distribution function shows that the 2*s* orbital penetrates more deeply into the 1*s* orbital than does the 2*p*.
- The weaker penetration of the 2*p* sublevel means that electrons in the 2*p* sublevel experience more repulsive force; they are more shielded from the attractive force of the nucleus.
- The deeper penetration of the 2*s* electrons means electrons in the 2*s* sublevel experience a greater attractive force to the nucleus and are not shielded as effectively.



Penetration

- The closer an electron is to the nucleus, the more attraction it experiences.
- The better an outer electron is at **penetrating** through the electron cloud of inner electrons, the more attraction it will have for the nucleus.
- The degree of penetration is related to the orbital's radial distribution function.
  - In particular, the distance the maxima of the function are from the nucleus

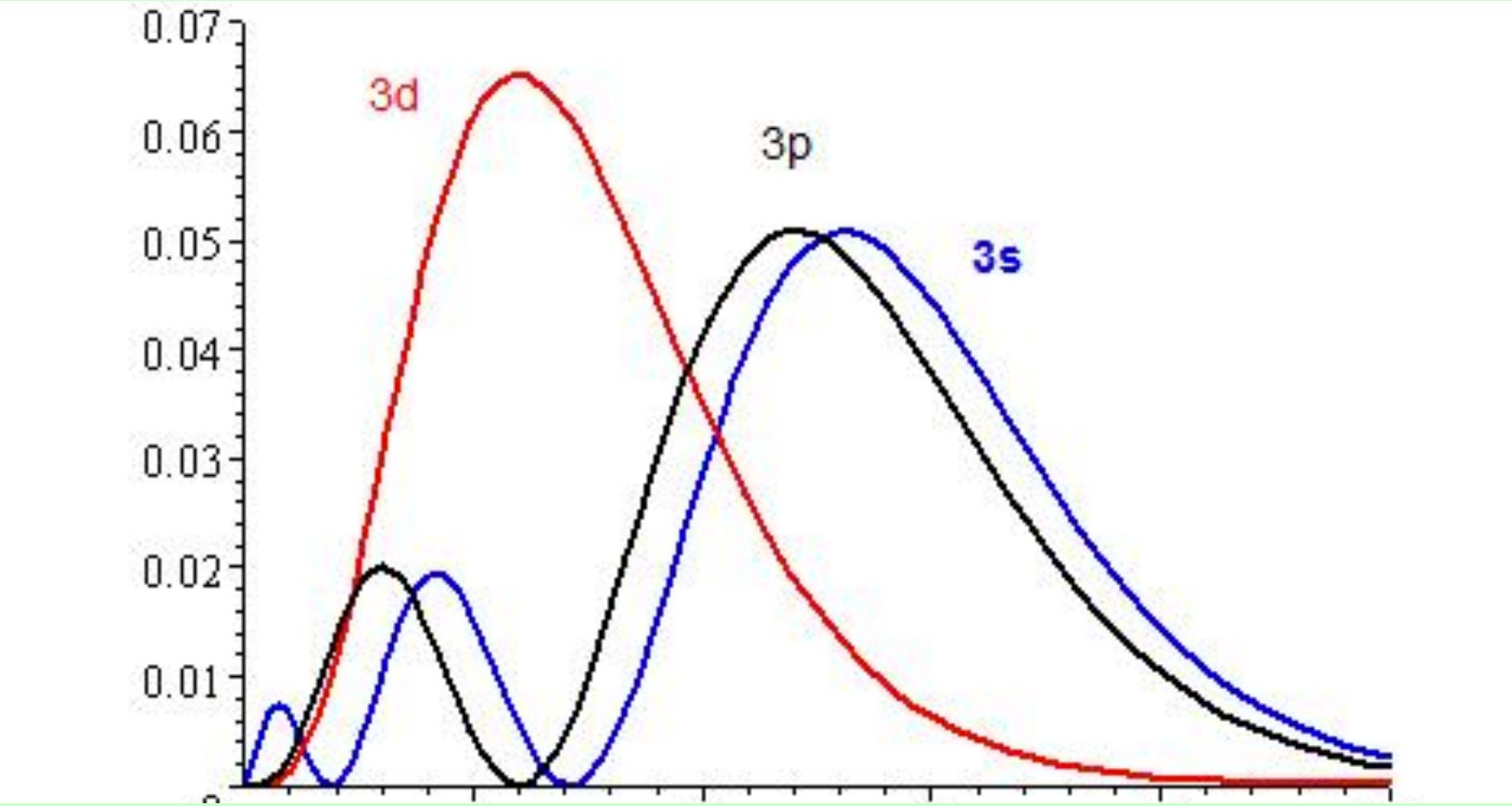
Orbitals in outer energy levels DO penetrate into lower energy levels. Penetration #1



This is a probability Distribution for a 3s orbital.

What parts of the diagram correspond to "nodes" – regions of zero probability?

Probability distribution



Probability distribution