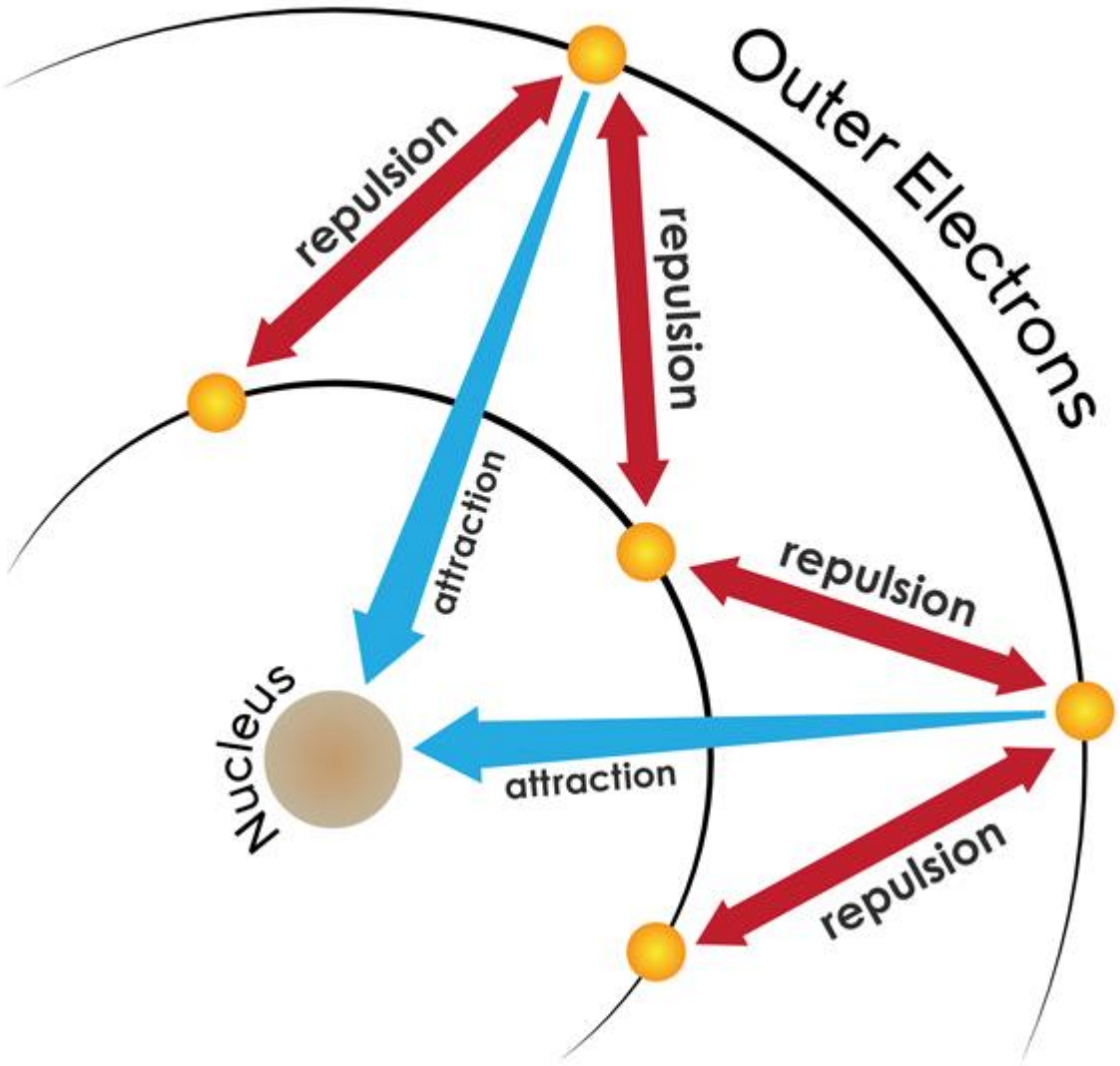
N17 – Atomic Structure and Periodicity

Shielding and Such

Shielding



In a multielectron system, electrons are *simultaneously:*

- Attracted to nucleus
- Repelled by each other.

Shielding

Outer electrons are shielded from nucleus by the core electrons.

- Shielding effect
- Outer electrons do not effectively screen for each other.

Shielding causes outer electrons to not experience the full strength of the nuclear charge.

- The electrons would be more attracted to the nucleus if the core electrons were not there!

Effective Nuclear Charge

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

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

Z = nuclear charge

S = number of electrons in lower energy levels.

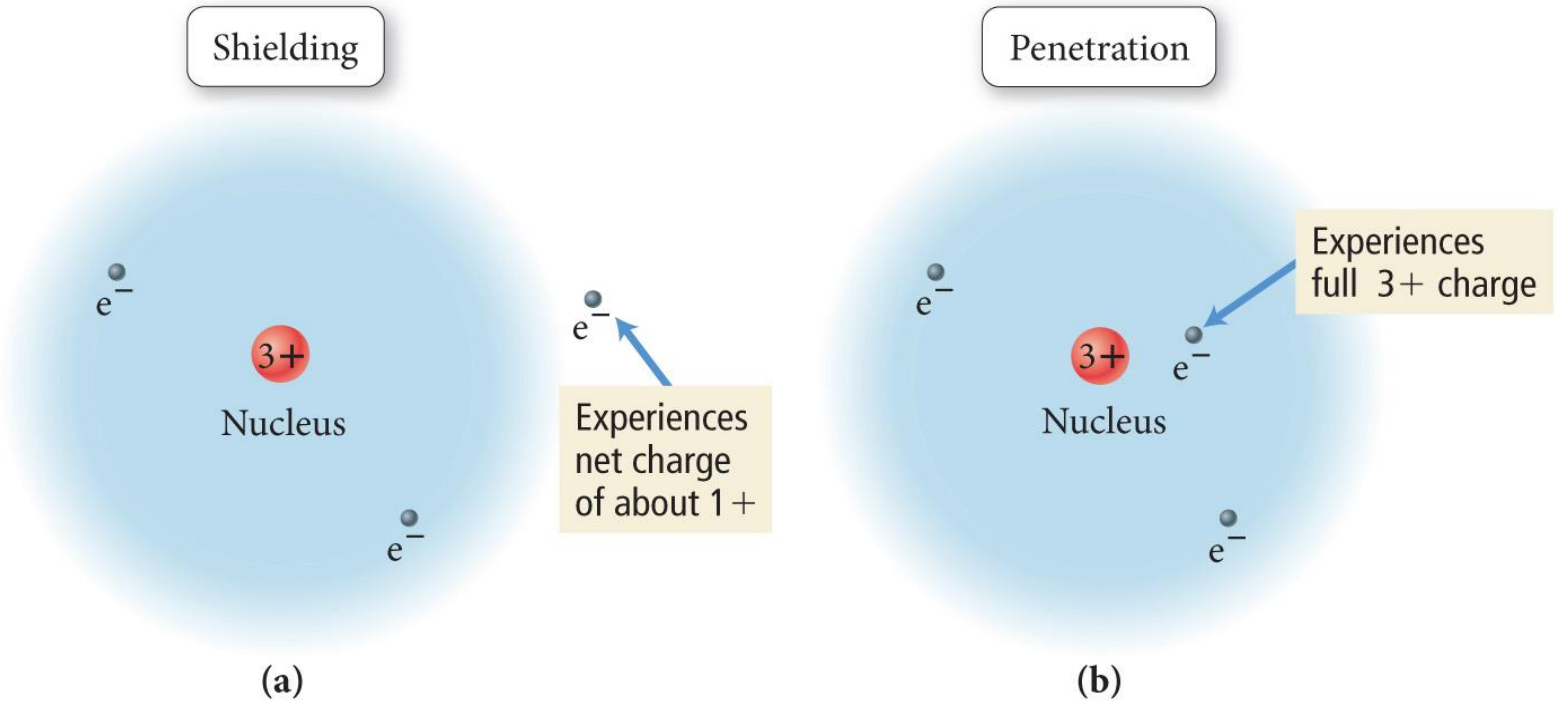
Electrons in the same energy level contribute to screening but since their contribution is so small they are not part of the calculation.

Trend in Shielding strength: *s* > *p* > *d* > *f*.

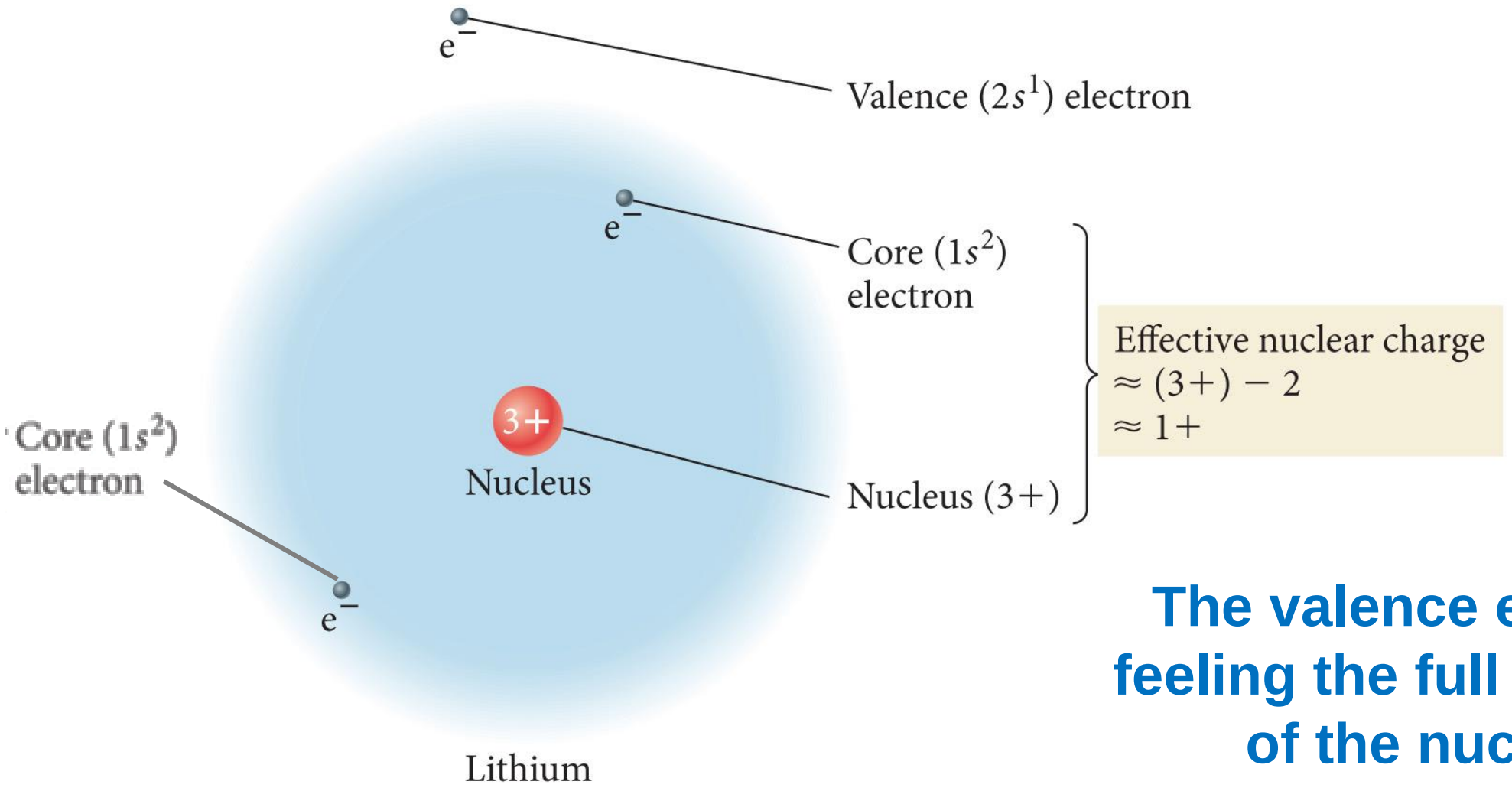
Shielding and Penetration

Penetration is when an electron spends time closer to the nucleus than it's outer boundary distance.

- Remember - there are different orbital shapes
- Some will have some electron density in closer to the nucleus than others



Shielding and Effective Nuclear Charge

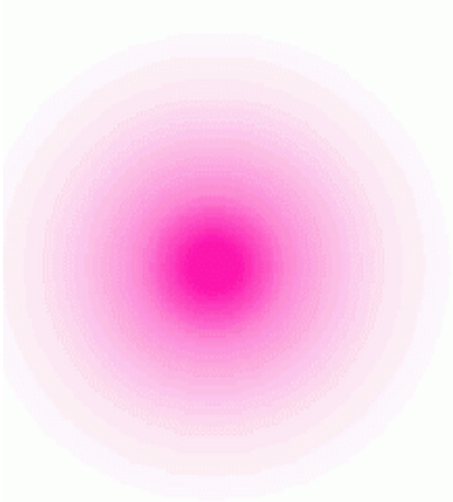


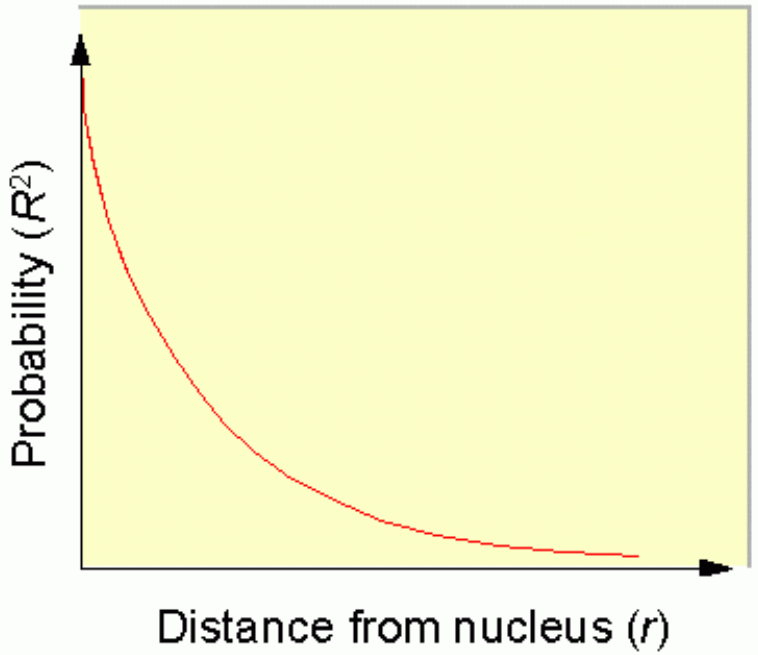
The valence e- is NOT feeling the full +3 charge of the nucleus!

Remember…

An orbital is a region within an atom where there is a probability of finding an electron. Orbital shapes are defined as the surface that contains 90% of the total electron probability.

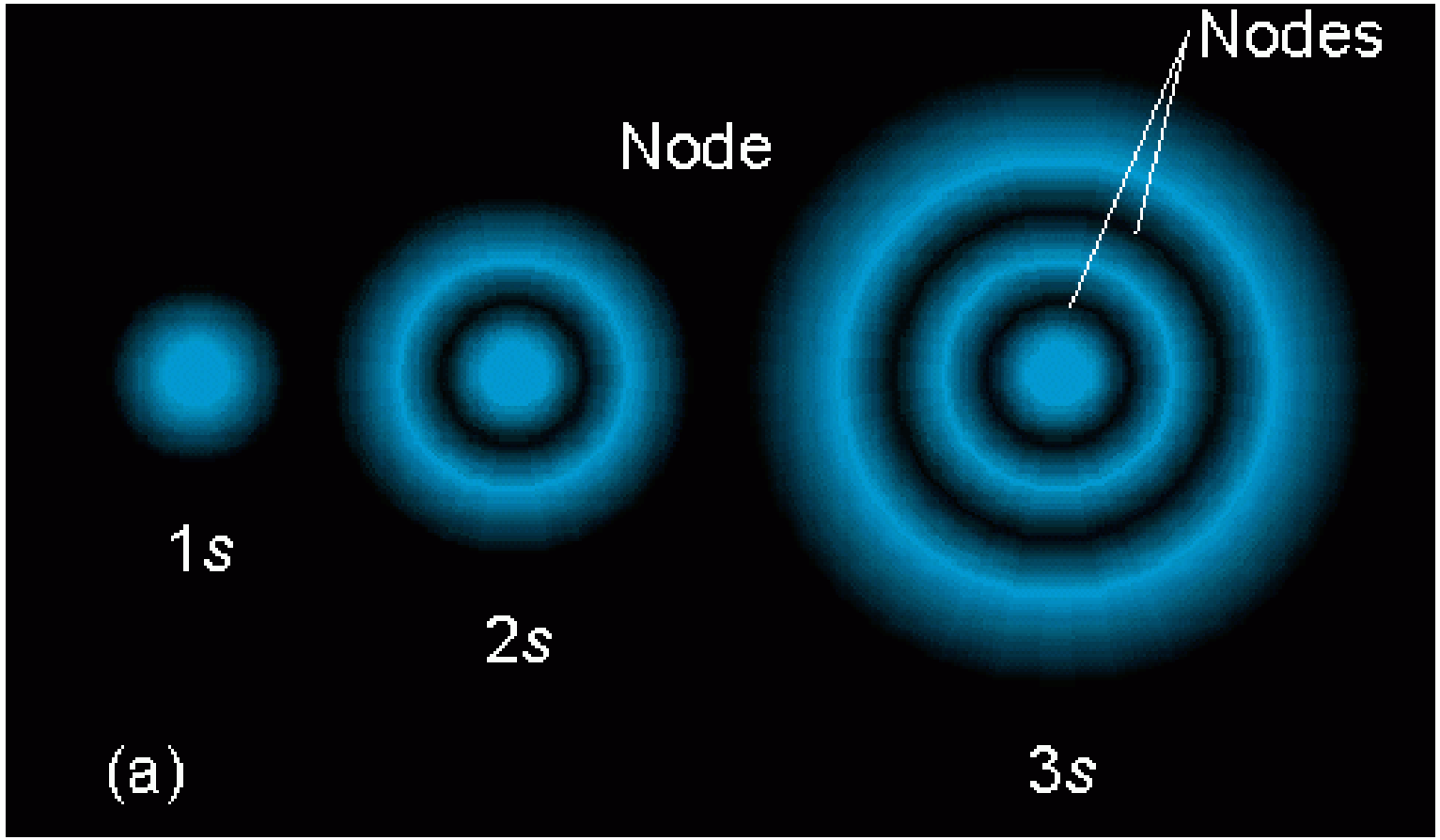
This is a probability diagram for the s orbital in the first energy level…





s Orbitals – not just a solid sphere!

s orbitals have areas of low probability inside them called nodes.



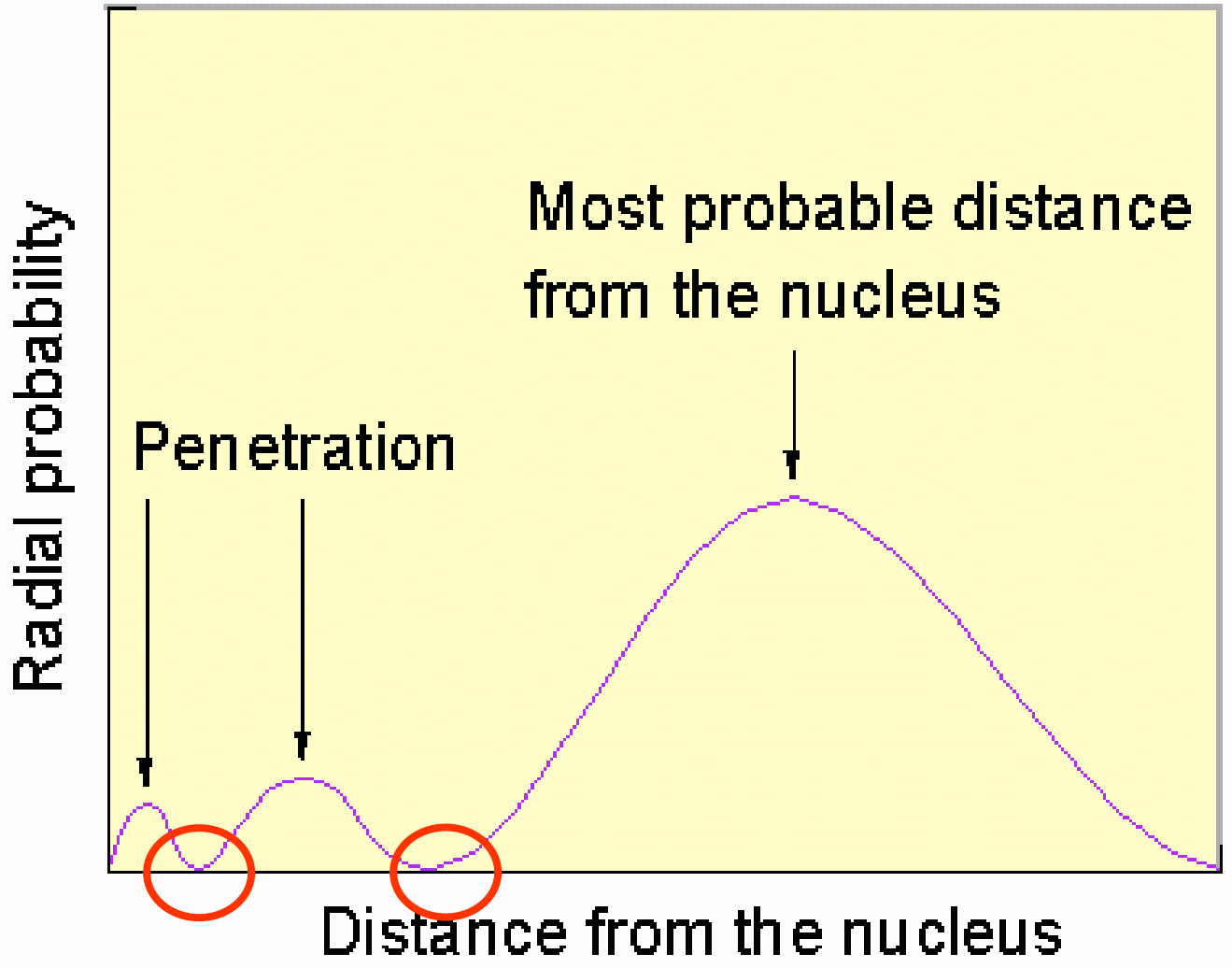
Penetration

Even larger s orbitals have some electron density near the nucleus!

Which s orbital is this?

3s orbital

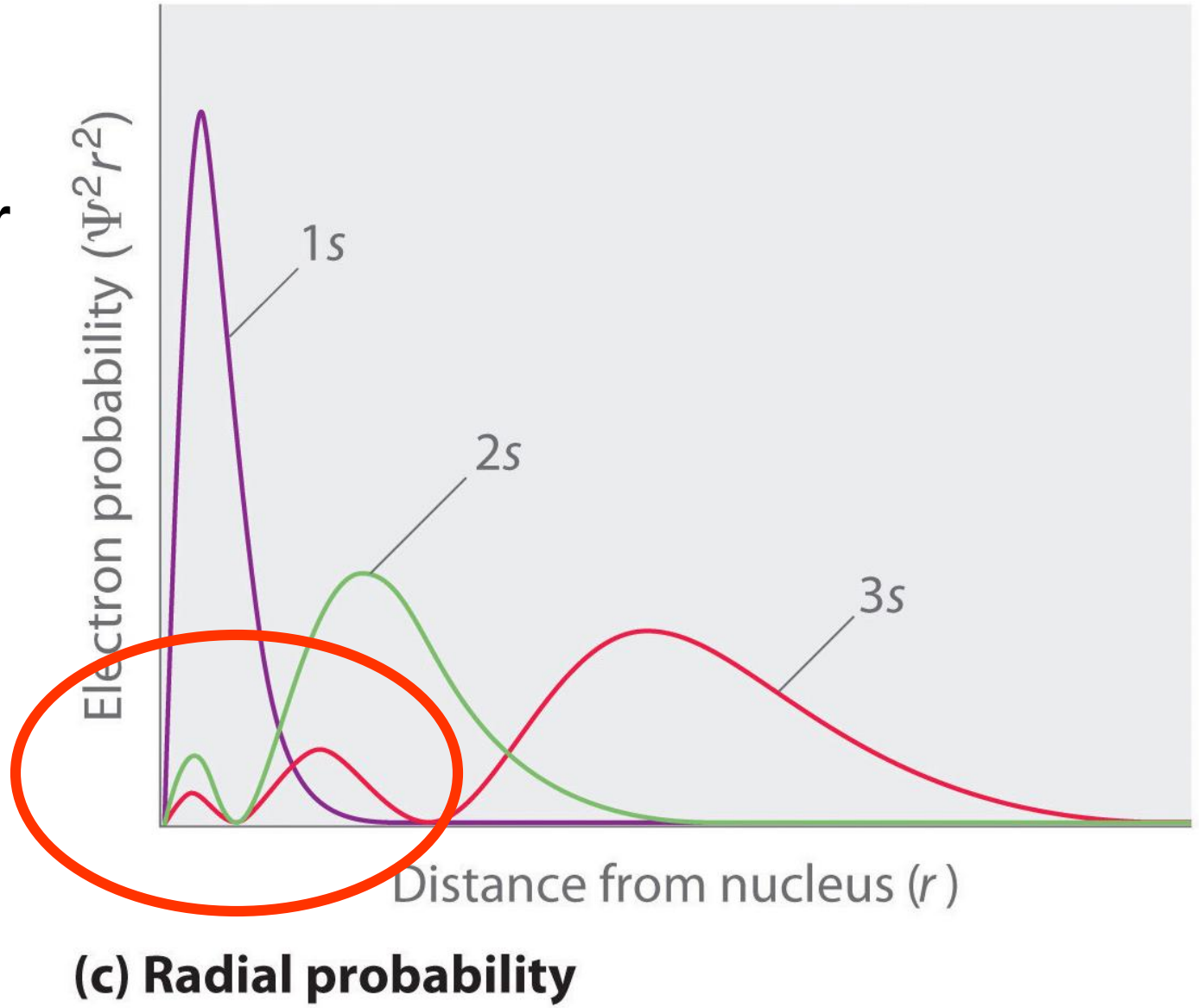
What parts correspond to the “nodes” – areas with zero probability?



Penetration

Even larger s orbitals have some electron density near the nucleus!

Penetration of the 2s electrons and the 3s electrons!



(c) Radial probability

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.

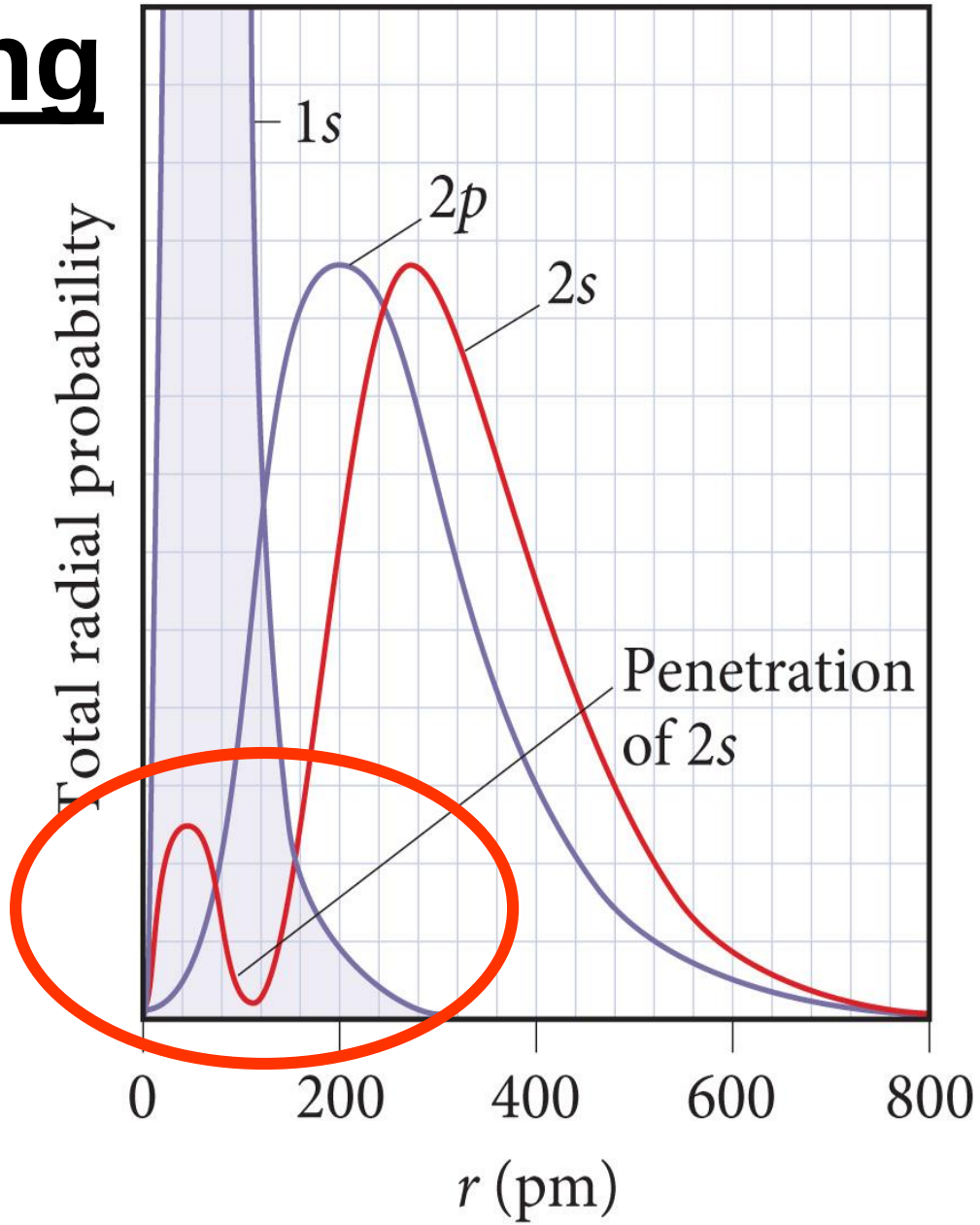
The degree of penetration is related to the orbital's radial distribution function.

Penetration and Shielding

- **2s orbital – penetrates more deeply into the 1s orbital, towards the nucleus than the 2p orbital does**

- **The weaker penetration of the 2p orbital means the 2p electrons experience LESS attractive force from the nucleus. They are more shielded from the nucleus.**

- **The greater penetration of the 2s means electrons in the 2s orbital experience MORE attractive force from the nucleus. They are less shielded from the nucleus.**



Careful…

We sometimes talk about shielding as meaning the core electrons are shielding the valence electrons from the nucleus

EXAMPLE: The s electrons shield more than the p electrons.
Ca experiences more shielding than Mg.

But sometimes we talk about shielding as electrons being shielded FROM the nuclear attractive forces

EXAMPLE: The p electrons are less shielded from the attractive force of the nucleus than s electrons because they do not penetrate towards the nucleus as much as the s electrons do.

Penetration, Attraction, Shielding

Penetration towards the nucleus:

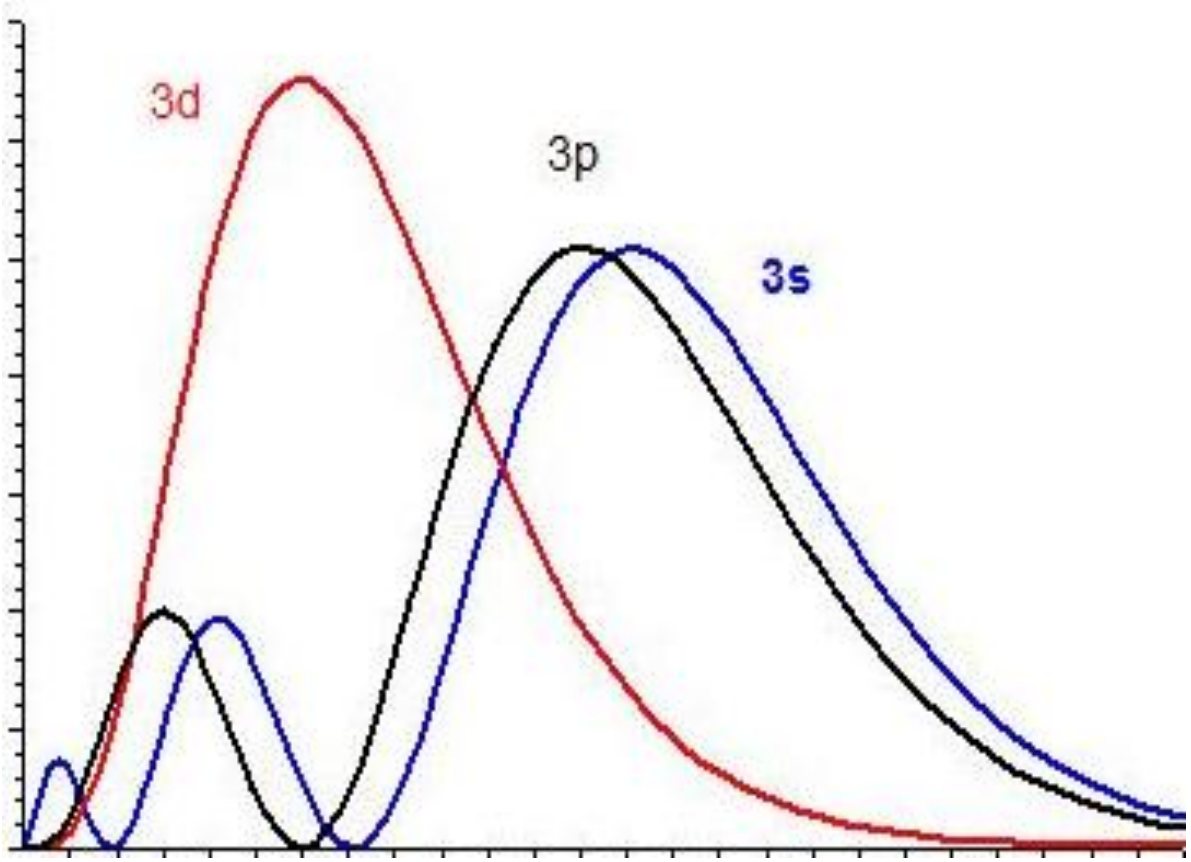
s > p > d > f

Attraction for nucleus:

s > p > d > f

Shielding they contribute for valence electrons:

s > p > d > f



Why care about shielding & penetration?

Helps explain periodic trends!

- **Zeff**
- **Ionization energies**
- **A lot of “exceptions” to the periodic trends patterns that we glossed over in Honors Chem**