Quiz 1

Please provide your class index number in addition to your full name.

1) In class, we discussed that for a Z-electron atom, we can approximate the potential felt by an electron using a central potential, which takes the following limits.

$$V_c(r) \simeq -\frac{e^2}{r} \quad \text{for large } r$$

$$V_c(r) \simeq -\frac{Ze^2}{r} \quad \text{for small } r$$

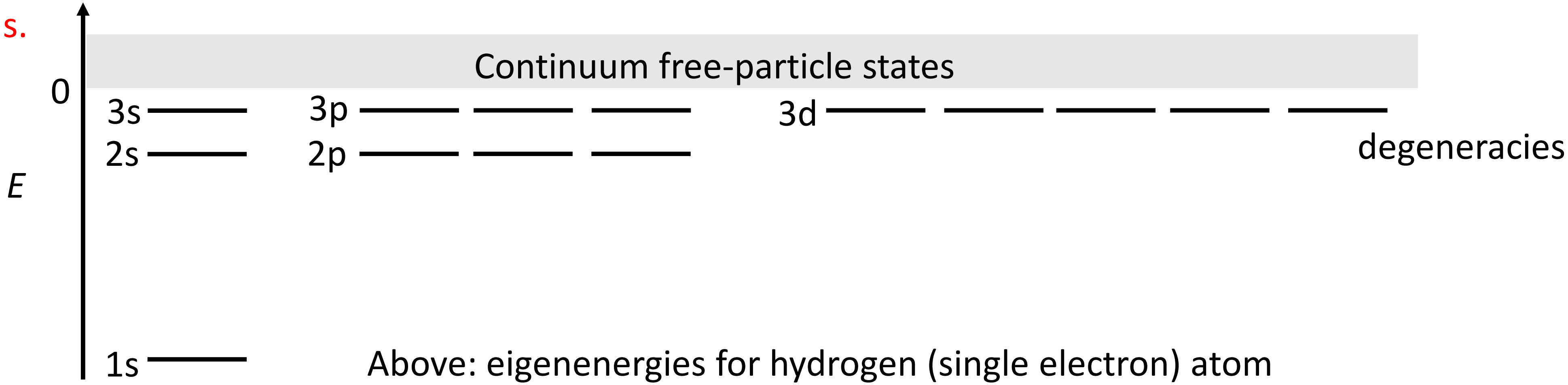
Answer the following questions using the single particle approximation and central potential approximation.

a) Given the single-particle spectrum for the H atom below, sketch a schematic of what the hierarchy of energy levels for 1s, 2s, 2p, 3s, 3p, and 3d orbitals might look like for a Ca atom (Z = 20).

b) Explain your answer.

Hint: Are states with the same quantum number l, with different m, still degenerate? How about states with the same quantum number n, different l?

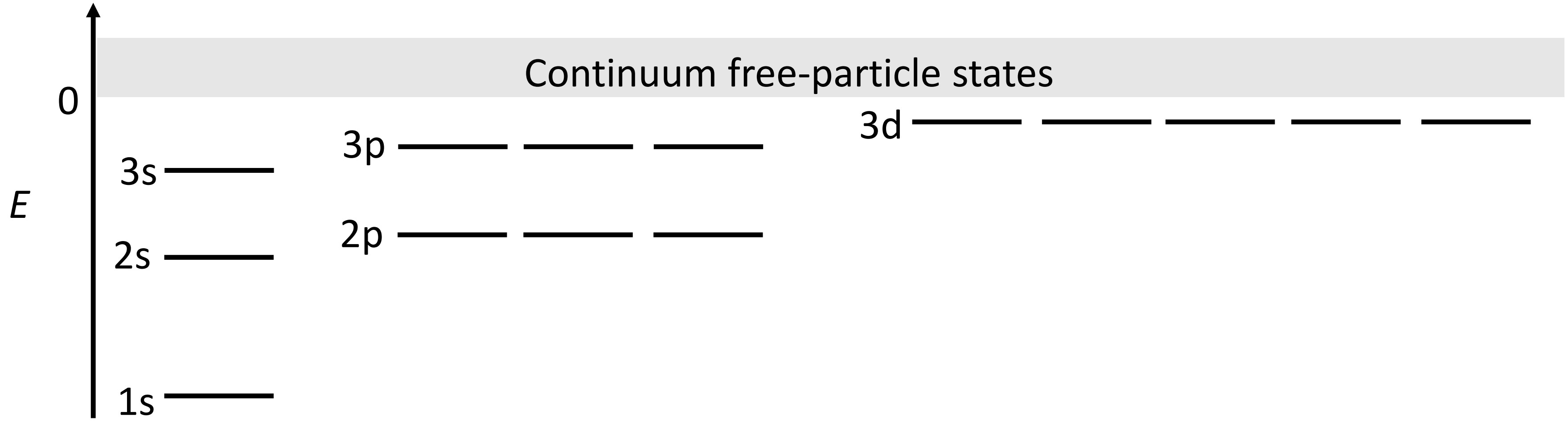
Also recall that there is a repulsive potential ~ $l(l+1)/r^2$; eg. s orbitals have a higher probability density near the nucleus than p and d orbitals.



Above: eigenenergies for hydrogen (single electron) atom

Eigenenergies for multi-electron atoms

1a)

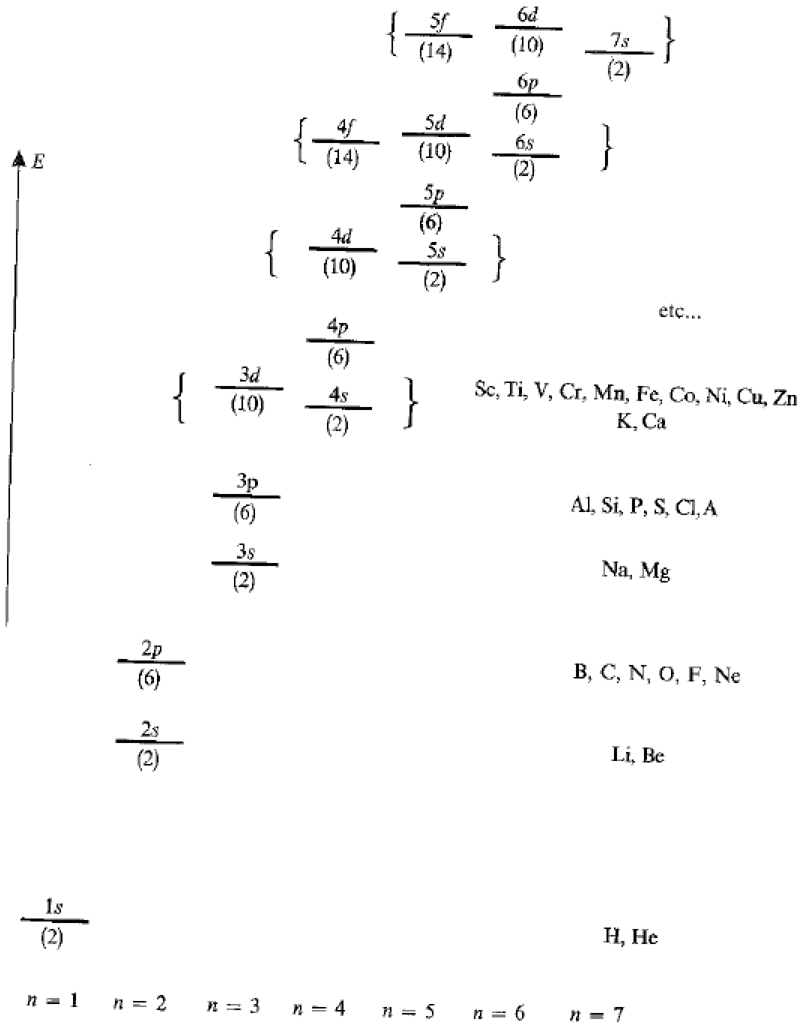


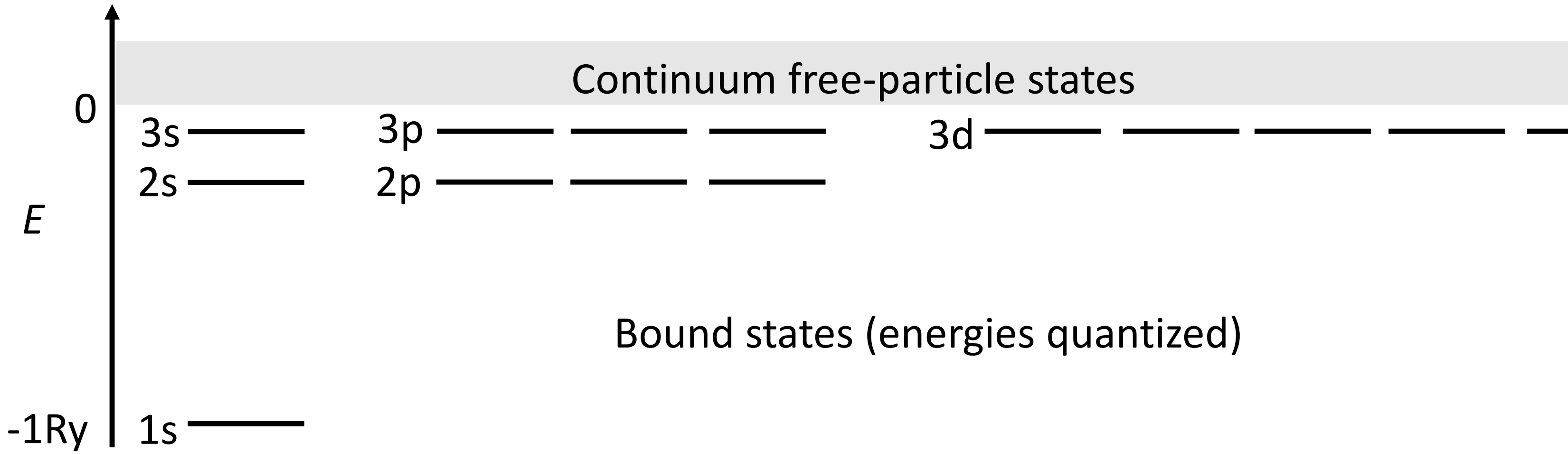
1b)

Compared to the hydrogen atom, the energy degeneracy is lifted for a given *n* but different *l* (eg. 2s is now more stable than 2p), because the 2p orbitals are less penetrating (farther from the nucleus than the 2s orbitals), due to the repulsive potential $l(l+1)/r^2$. While <u>in the H atom, the 2s and 2p orbitals have the same energy</u>, <u>the screening from other electrons in a multi-electron atom further weakens the strength of the Coulomb attraction felt by the 2p electron compared to the 2s electron</u>. Therefore, the 2p orbital energy is now higher than the 2s orbital energy. Similar for the 3s, 3p and 3d orbital energies.

Orbitals with the same quantum number l but different quantum number m are still degenerate, because the Hamiltonian does not depend on m.

Eigenenergies for multi-electron atoms





Above: eigenenergies for hydrogen (single electron) atom

- Compared to the hydrogen atom, we see that the energy degeneracy is lifted for a given *n* (eg. 2s is now more stable than 2p)
- Also we see that 4s is more stable than 3p.

From Cohen-Tannoudji

Points to note

- In general, stronger attraction stabilizes the electron, implying a more negative energy for the single particle state.

- We can also use the term “shielding” instead of “screening”.