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English CPH E-Book

Theory of CPH

Section Ten

Effective Nuclear Charge

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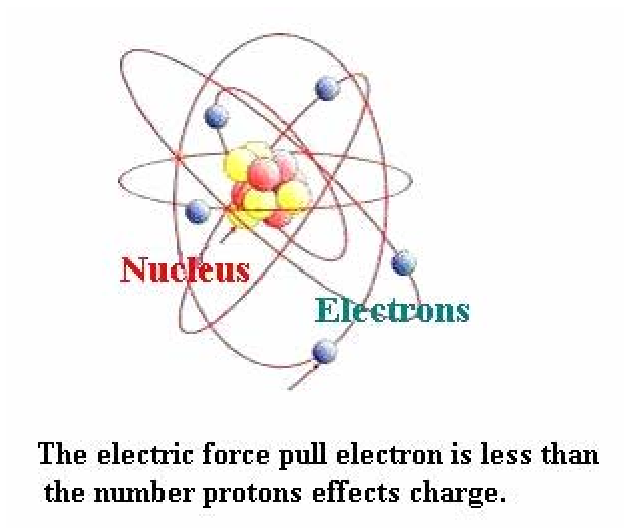
Contains:

Introduction:
The effective nuclear charge is the "pull" that the specific electron "feels" from the nucleus.
Example; hydrogen atom contains one proton and one electron. The effective nuclear charge on electron is equal 1 in hydrogen atom. Helium contains two protons and two electrons. But there is not the effective nuclear charge equal 2 on each electron in helium atom, it is about 1.7 units.
There is some rules for calculation the effective nuclear charge in modern physics. But there are not analyses about it.
According CPH Theory it is explainable how nuclear charge loses in its path from nucleus to electrons.



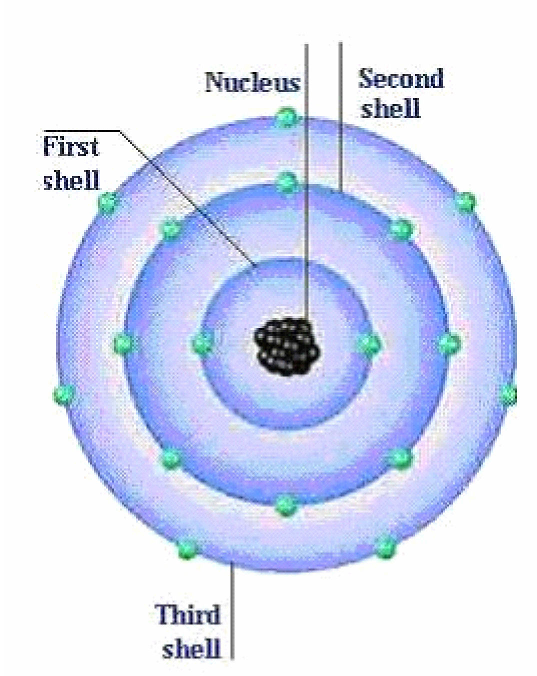
Staler Rule;
Of the first time, Slater had give a simple rule for calculate the effective nuclear charge on any electron in any atom. Specifically, Slater's Rule determines the shielding constant which is represented by S. To determine the effective nuclear charge use this equation:

$$Z^*=Z-S$$

Where Z* is effective nuclear charge Z atomic number.

According Staler rule you must order the configuration differently then what you are used to. Group each electron like this:

(1s)(2s,2p)(3s,3p)(3d)(4s,4p)(4d)(4f)(5s,5p)(5d)(5f)...



Electrons to the right of the electron you have chosen do not contribute because they don't shield. In the same group, each electron shields 0.35.

For 1s	S=0.3
For electron in s or p, when n>1	$S = 1.00\ N_2 + 0.85\ N_1 + 0.35\ N_0$

N_2	N_1	N_0
Electrons in n-2	Electrons in n-1	Electrons in calculation orbit

Example: As from a 3d perspective (Its nuclear has 33 protons);

$1s^2$	2x1=2
$2s^2$, $2p^6$	8x1=8
$3s^2$, $3p^6$	8x.85=6.8
$2d^{10}$	10x0.35=3.5
Total	S=20.3

Z*=Z-S=33-20.3=12.7

Clementi and Raimondi;
Clementi and Raimondi did their work on effective nuclear charges in the early 1960s. By this time, there was a great deal of background work that had been done on orbital and molecules. And the computer had been invented! This gave them the ability to incorporate self-consistent field (SCF) wave functions for the hydrogen to krypton atoms into their calculations. They didn't have to rely on Slater-type orbital which, for simplicity of calculation, didn't contain nodes.
They were thus able to go to a greater depth with a refined mathematical model, and this allowed
Them for clearly distinguish the s-orbital from the p-orbital in determining their set of rules. Specifically, they had a better model for dealing with electron penetration of the inner core.
The results of Clementi's method are difference of Staler's rule. For example Clementi calculated for As atom from a 3d perspective Z*=17.378 (Staler's is equal 12.7).

There are no analyses
Staler's rule and Clementi's method based on experiments. There is no any analytic concept why and how the strongly of nuclear charge does lose? The effective nuclear charge leads we have a new looking on force and relationship between force and energy. Is force perishable? If force is not perishable, why the effective of nuclear charge does change of an orbit to other orbit? What happens for the strongly of nuclear charge in during its traveling toward electrons? Is force convertible? If force is convertible, it does convert to what? When an electron accelerates toward a proton, then energy of electron does increase. Question is that; what happens for the amount of force? According CPH theory force and energy are convertible. Force converts to energy and energy changes to force. I will explain the effective nuclear charge by CPH theory.

Work is quantized;
Theoretical physics and evidence show energy is quantized. Also, when force applied on a particle/object, energy of particle/object does change. Relations;

$$Fdx = -dU \text{ and } W = \mathbf{F}.\mathbf{d} = \Delta E = \Delta mc^2$$

Show if energy is quantized then work can not be continually. When a photon is falling in a gravitational field, its energy does increase. But energy of photon is quantized. So, work of gravity force must be quantized. Also, when an electron accelerates in an electrical field, the energy of electron does change. But energy of electron is quantized, so work of electrical force is quantized too. But d (distance) is continually, so F (gravity force or electric force) is quantized.
How we can define a quantum of force? Before we define a quantum of force, we must define a quantum of work. So, we need select a short length for that. I propose Lp (Planck Length) for that. It is equal;
Lp=1.6x10 power minus 35 m.

Also, I defined a quantum of gravity force (in CPH Theory) Fg, that is equal;
So, a quantum of work is

$$Wq=\mathbf{F}g.\mathbf{L}p$$

And at usual case W=nWq, n is an integer number. (n=...-2, -1, 0, 1, 2...)

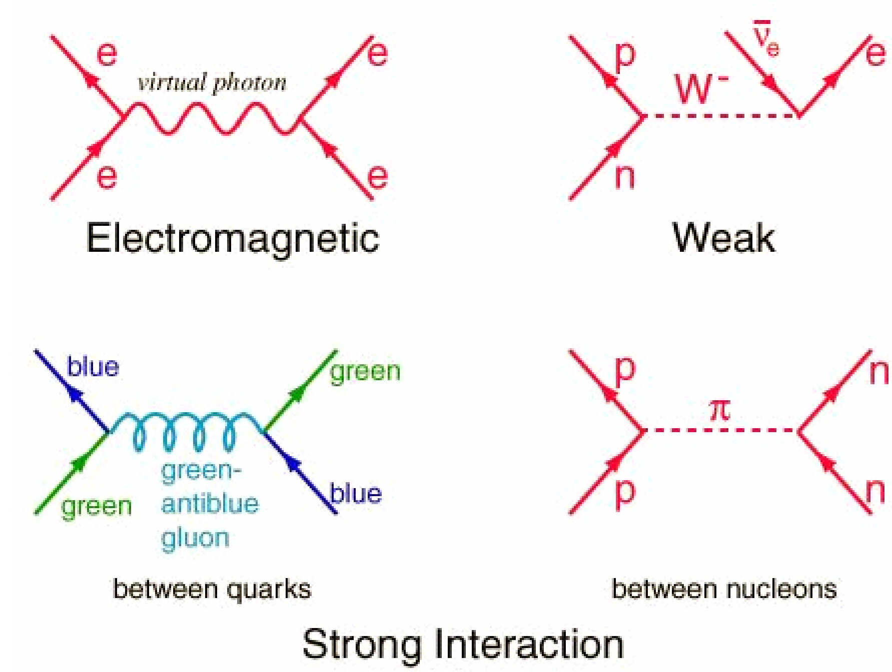
Force and Energy are convertible to each other;
I take a shot with mass m. I shoot it with velocity v upward the earth. Shot takes kinetic energy. In during shot is traveling upward, gravity force works on it. Gravity work is negative, and shot's energy does decrease until shot does stop. Then shot falls toward the earth and its kinetic energy increases.
When shot is moving upward, it loses energy equal $1/2mv^2$ that it is equal $1/2mv^2=nFgLp$, and shot's energy converts to n quantum gravity force. Also, when shot is falling n quantum gravity force converts to kinetic energy. We are not able show the intensity of gravity increases and decreases by moving a shot in gravitational field. But effective nuclear charge shows force loses in its path.

Exchange Particles in Quantum Theory

All elementary particles are either bosons or fermions (depending on their spin). The spin-statistics theorem identifies the resulting quantum statistics that differentiate fermions and bosons.

Interaction of virtual bosons with real fermions is called fundamental interactions. Momentum conservation in these interactions mathematically results in all forces we know. The bosons involved in these interactions are called gauge bosons - such as the W vector bosons of the weak force, the gluons of the strong force, the photons of the electromagnetic force, and (in theory) the graviton of the gravitational force.

In particle physics, **gluons** are vector gauge bosons that mediate strong color charge interactions of quarks in quantum chromodynamics (QCD). Unlike the neutral photon of quantum electrodynamics (QED), gluons themselves participate in strong interactions. The gluon has the ability to do this as it itself carries the colour charge and so interacts with itself, making QCD significantly harder to analyze than QED.



Since gluons themselves carry color charge (again, unlike the photon which is electrically neutral), they participate in strong interactions. These gluon-gluon interactions constrain color fields to string-like objects called "flux tubes", which exert constant force when stretched. Due to this force, quarks are confined within composite particles called hadrons. This effectively limits the range of the strong interaction to 10^{-15} meters, roughly the size of an atomic nucleus.

The photon is the exchange particle responsible for the electromagnetic force. The force between two electrons can be visualized in terms of a Feynman diagram as shown below. The infinite range of the electromagnetic force is owed to the zero rest mass of the photon. While the photon has zero rest mass, it has finite momentum, exhibits deflection by a gravity field, and can exert a force.

Feynman diagram for the electromagnetic force between two charges.

The photon has an intrinsic angular momentum or "spin" of 1, so that the electron transitions which emit a photon must result in a net change of 1 in the angular momentum of the system. This is one of the "selection rules" for electron transitions

Exchange Particle in CPH Theory

As I told before particle charges use color-charges that exist in perimeter produce **virtual photons.** Electron produces negative virtual photon and proton produces positive virtual photon. So, they put out electricity fields around themselves.

Now look at two charge particle with different sign (an electron and a proton). Proton emits positive virtual photons. Photon moves toward the electron. Electron absorbs it. When photon enters into structure of electron, charge of electron does unbalance. So, electron does decay virtual photon to positive color charge toward the proton. But positive color-charges have positive effect charge, they were pulling electron beyond themselves. The same case happens for proton and negative virtual photon. And they (electron and proton) absorb each other. Any electrical interaction does like this.

Now suppose a charge particle accelerates in electric field and its velocity does change. When energy of electron increases, electric force converts to energy. And when energy of electron decreases, energy does convert to electric force.

Effective nuclear charge in CPH Theory;

Current of electric force is like of gravity force's current. Difference between them is in the heir's strongly. Suppose an atom contains n protons and n electrons. Electrons are rotating in their orbits around nucleus. Electron B is between nucleus and electron A. Given Fe is a quantum of electric force. Now suppose n1 electric force particles start their travel of nucleus toward electron A. n1=kn, n is number of protons in nucleus and k is a natural number. When these electric force particles reach to electron B, they work on it. (B is between nucleus and electron A). Then n2 electric force particles convert to energy, and energy of electron B does change. So, (n1-n2) electric force particles reach to electron A, and effective nuclear charge on A is equal Z*=Fe(n1-n2). Then electron A feels F=(n1-n2)Fe of nucleus. If there were electrons B, C, D... between nucleus and electron A, then n2, n3, n4 .. Convert to energy and [n1-(n2+n3+n4...)] reach to A. Then A feels effective nuclear equal Z*=Fe[n1-(n2+n3+n4...)].

When n1=n2+n3+n4..., then electron A never feels any effect of nuclear charge.

Let come back to electron B and see what happened for it. When n2 electric force particles reach to B, B's energy changes, and it leaves its orbit. But B is not alone and other electrons and nucleus have effect on electron B. They do return B to its orbit. And its energy converts to force, this interaction is continually.

Atom's orbits;

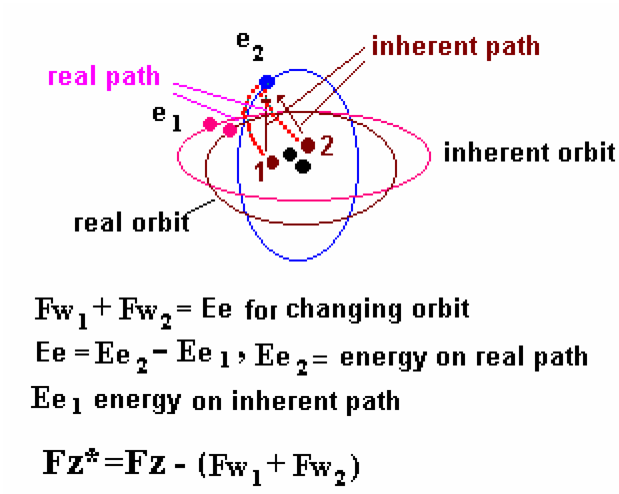
If external forces that applied on an electron was being constant, then its energy and orbit is stable. But the strongly (and directions) of electric forces that applied on any electrons does change continually. So, energy of electron (and direction) is not constant and its velocity and orbit do change speedy. Also, the magnetic field of electron does change continually. So, this changing of magnetic field has effect on other electrons and nucleus. The spin and volume of nucleus do change, and it has effect on electrons and their orbits. So, electron oscillates around its orbit.

Examples;

Suppose two objects A and B absorb each other. By according CPH Theory a force particle leaves A and pulls it toward B, when force particle reaches to B, another leaves B and pulls it toward A and so on. In the following examples please attend that electrons are moving in their orbits, but Fz (nuclear charge) moves faster than electrons.

Hydrogen;
Hydrogen atom contains one proton and one electron in 1s, so Fw=o and Fz=Fz*. Because there is no any other electron in hydrogen atom and Fw=0. Clementi supposed Fz*=1

Helium;
Helium contains two protons and two electrons in 1s. Fz=2 from two protons moves toward electron1. Electron2 has electric charge and magnetic field. So, Fz acts on electron2. But direction of Fz is toward the electron1. So, electron2 does change direction of Fz. It depends to distance between electrons in this orbit. Suppose this effect is nothing.
But, Fz works on electron2, energy of electron2 increases and Fz loses a part of its strong. So, the effective nuclear charge Fz* on electron1 given by;
Fz*=Fz - Fw



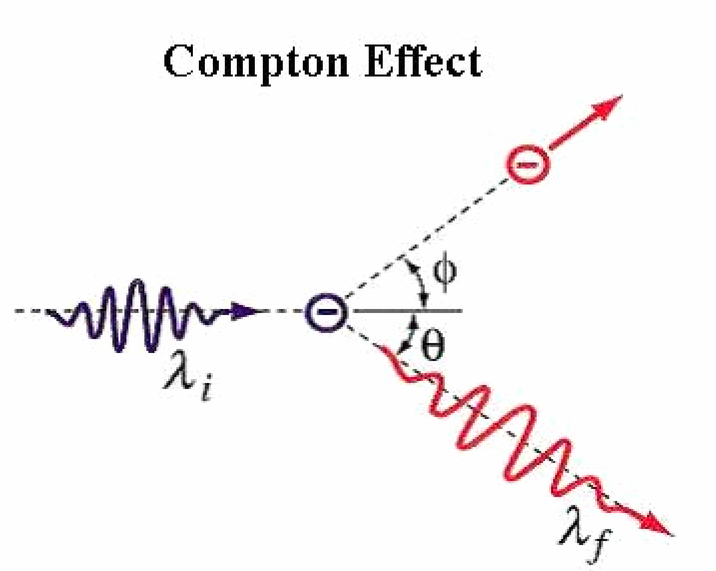
Energy of electron2 increases equal E=W. It leaves its orbit. But electric force leaves it toward nuclear and pulls electron2 toward nuclear. Also, electric force of electron1 acts on it. Then electron2 comes back to its orbit and loses energy E, and E converts to electric force equal Fw. Then Fw does add to Fz* that is coming back of electron1 and Fz=Fz*+Fw reaches to nuclear. So, nuclear feels that effective force of electron1 is equal Fz.
The effective nuclear charge Fz* on electron2 is same as electron1. By according Clementi calculate Fz*=1.688

Lithium;
Lithium has 3 protons and 3 electrons, two electrons are in 1s and one electron is in 2s.

For 1s;
Fz=3 from 3 protons moves toward electron1 in 1s orbit. This case is same as Helium, but radius of 1s orbits is smaller than in Helium and distance between electrons is less than Helium's orbit. So deviation direction of Fz is less than in Helium. It shows the effect of deviation direction for Fz is less than Helium. By according Clementi's calculate Fz*=2.691. Do compare with Helium that Fz*=1.688.

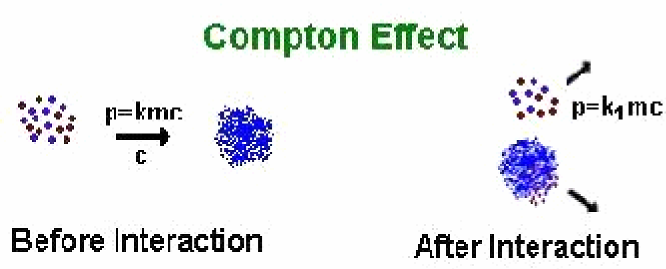
For 2s;
There is one electron in orbit 2s in Lithium. So, this electron feels Fz* that is coming of over the orbit 1s. Fz=3 leaves nuclear toward it. Fz works on two electrons in orbit 1s. Fz loses Fw1 for act on electron1, and Fw2 for act on electron2. So, when Fz reaches to orbit 1s, It comes up to F'z=Fz - (Fw1+Fw2).
In during F'z is passing of orbit 1s, it works on the sum of electron1 and electron2. Suppose this work is equal Fw3.
So, Fw=Fw1+Fw2+Fw3 and Fz*=Fz-Fw reaches to electron in orbit 2s. By according Clementi's calculation Fz*=1.279.
When Fz* reaches to electron, then another electric force particle equal Fz* leaves it toward nuclear. When it does reach to 1s orbit, it works on that. In during Fz* is passing of orbit 1s, energy E=W converts to force Fw and Fz=Fz*+Fw reaches to nuclear.

Compton Effect in Atom;
Effective nuclear charge is like Compton Effect. In Compton effect, photon loses energy and electron takes energy.



According CPH Theory in Compton Effect a number color-charge and magnetic-color leave photon and enter into electron. Effective nuclear is like it, in a difference.

Photon is formed of positive color-charge, negative color charge and magnetic-color that make electromagnetic energy. So, electron keeps energy.
But **virtual photon** is formed of negative (or positive) color-charges.
And electron cannot keeps color-charge and loses speedy.



Question is that;
Gravity has effective force like effective nuclear charge?

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