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Studying Of Binding Energy Of Electrons In Multi Electrons Atoms By Fermi-Statistics

دراسة طاقة الترابط للالكترونات في الذرات متعددة الالكترونات باستخدام إحصائيات-فيرمي

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Abstract:

The method of finding binding energy for electrons in atoms has many difficulties, because there are many mathematical difficulties in it. Up today the problem isn't solve completely and explicitly except for H-atom and for ions like it i.e. the ions have one electron in the outer orbit. To find of He-atom every theories an approximation method to find it. To find the binding energy in multi electrons atom for example (U_{92}) need to solve a system of (92) partial differential equations with (276) independent variable and its impossible to do that, it has been found the binding energy for H-atom in the early days of quantum mechanics. It has been put an equation for the binding energy of H-atom.

Also it has been found an approximate equations for binding energy for He-atom and Li-atom by (Born) by a method called (Born approximation method) it has been reached to a results near to experimental results. It has been found binding energy for large number of atoms approximately in many scientific research institutes. (Hartree, fock, Rothaan).

الخلاصة :

ان عملية إيجاد طاقة الالكترونات في الذرة هي من أصعب العمليات حيث تكتنف الموضوع صعوبات رياضية جمة بحيث لم يتم حل المسالة بشكل دقيق الا بالنسبة الى ذرة الهيدروجين او الايونات المتشابهة لذرة الهيدروجين أي الايونات التي تحتوي إلكترون واحد في المدار الخارجي اما عملية إيجاد طاقة ذرة الهليوم فقد تم اللجوء فيها الى التقريب ان عملية إيجاد طاقة الالكترونات في الذرات المتعددة الالكترونات مثلا (U_{92}) يستلزم حل نظام مكون من (92) من المعادلات التفاضلية الجزئية وتصل (276) متغير وهذه عملية مستحيلة لحد الآن.

لقد تم إيجاد طاقة الترابط للهيدروجين في المراحل الأولى من تاريخ ميكانيك الكم حيث تم وضع معادلة تعطي طاقة الإلكترون في ذرة الهيدروجين وتم إيجاد طاقة الترابط للهليوم ولليثيوم بمعادلات تقريبية من قبل (Born) بما يسمى بطريقة بورن للتقريب (Born approximation method) وتم الوصول الى نتائج مقاربة الى الواقع بشكل كبير جدا.

وقد تم إيجاد طاقة الترابط لعدد من الذرات بطريقة تقريبية في كثير من مؤسسات البحث العلمي ومن قبل علماء مثل (Hartree, Fock, and ploothaan) في هذا البحث استخدمنا طريقة إحصائية في إيجاد معادلة لطاقة الترابط للعناصر الثقيلة لذلك فان المعادلة المستنتجة هي إحصائية بطبيعتها وتكون أكثر انطباقا على الواقع كلما كانت الذرة أثقل أي عدد الالكترونات اكبر. .

Introduction:

The quantum mechanical methods mode its possible to describe any system composed from electrons atoms or molecules. But there is a difficulty in solving the equations conserved to that system although to atom have tow electrons. This difficulty is so large that there is no one solved this problem up to now[1].

It has been used the approximation methods in this problem. But we can use some laws to describe the general motion that don't needs the knowledge of the wave function for it (ψ).

The method which is applied in this research is the statistical method (Fermi distribution) that can be applied to particles have spin equals to (1/2 ħ). We found the most important physical quantity.

In this research we used statistical method to find an equation to find the binding energy for heavy elements. So the results of the equation are more acceptable with the experimental results for more large atomic number (Z) i.e. the binding energy of the electrons the binding energy has been calculated for many elements.

Theory:

Fermi distribution:

Its well known to find the binding energy for electrons contracts with each other, we should use Fermi distribution that can be applied to particles have spin equals to (1/2 ħ).
We can write the (Fermi distribution law)[2]:

$$dn(\varepsilon) = \frac{V(2m^3)^{1/2}\varepsilon^{1/2}\,d\varepsilon}{\pi^2 h^3} \cdot \frac{1}{e^{\frac{\varepsilon-\mu}{\theta}}+1} \quad \text{.....(1)}$$

Where dn(ε) is the total number of status have energy between (ε) and (ε + dε), (θ) is thermal degree in (erg.), (C^0=11200× θ) thermal degree in centigrade, μ is constant have energy unit, m is the mass of electron, (h) is Plank constant, the factor $\left(\frac{1}{e^{\frac{\varepsilon-\mu}{\theta}}+1}\right)$ give the probability that the states are occupied by electrons we can look to f(ε)= $\left(\frac{1}{e^{\frac{\varepsilon-\mu}{\theta}}+1}\right)$ as a probability or the mean number of particle because the value of f(ε) is between Zero and one [2].
Its known from quantum mechanic that the number of particle have energy from Zero→ε_0 can be give by the equation [3]:

$$N = \frac{V(2m^3)^{1/2}}{\pi^2 h^3}\int_0^{\varepsilon_0}\varepsilon^{1/2}\,d\varepsilon = \frac{V(2m^3)^{3/2}\varepsilon^{3/2}}{3\pi^2 h^3} \quad \text{.....(2)}$$

(V_i) is the volume occupied by electrons, (m_i) is the mass of electrons. If g(ε) is a function of the number of states have the same energy, the energy for all states have energy between Zero and (ε)

$$E = \int_0^{\varepsilon} \varepsilon\; dg(\varepsilon) \quad \text{.....(3)}$$

We have

$$E = \int_0^{\varepsilon_0} N\; d\varepsilon = \int_0^{\varepsilon_0} \frac{V(2m^3)^{3/2}\varepsilon^{3/2}}{3\pi^2 h^3}\,d\varepsilon$$

$$= \frac{V(2m)^{3/2}\varepsilon_0^{\,5/2}}{5\pi^2 h^3} \quad \text{.....(4)}$$

The equation of Homogenous field:

There is an equation between energy and the density of electric charge:

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\varphi}{dr}=4\pi en.....(5)$$

[n= dN/dV= electrons density], (φ) is the potential. There is an equation in statistical physics between (n) and (φ).

$$(3\pi^2)^{2/3}\frac{h^3}{2m}(n)^{2/3}=\varepsilon_0=e\varphi.....(6)$$

Substitute (n) from (5) in (6) we obtain:

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\varphi}{dr}=\frac{2^{7/2}}{3\pi}\frac{m^{3/2}}{h^3}e^{3/2}\varphi^{3/2}.....(7)$$

Let us take the function (ψ) related to (φ) by the equation: $(\varphi=\frac{Ze}{r}\psi)$.

The function (ψ) is dimensionless because $(\frac{Ze}{r})$ have units of potential. substitute (ψ) in (7):

$$\frac{d^2\psi}{dr^2}=\frac{2^{7/2}}{3\pi}Z^{1/2}\frac{m^{3/2}}{h^3}e^3\frac{\psi^{3/2}}{r^{3/2}}.....(8)$$

Let us take another independent variable (x) in such a way that:

$$r=(\frac{3\pi}{2})^{7/2}\frac{1}{Z^{1/3}}\frac{h^2}{me^2}x.....(9)$$

We obtain the equation:

$$\frac{d^2\psi}{dx^2}=\frac{\psi^{3/2}}{x^{3/2}}.....(10)$$

Calculation of electron energy in atom:

The kinetic energy for electrons in atom is:

$$E_k=\int_0^\infty \varepsilon n\,dV=\int_0^\infty\frac{(2m)^{3/2}}{5\pi^2h^3}\varepsilon^{5/2}4\pi r^2\,dr$$

$$=\frac{(2m)^{3/2}}{5\pi^2h^3}4\pi\int_0^\infty(e\varphi)^{5/2}r^2\,dr.....(11)$$

For the limit of kinetic energy in equation is the potential energy (eφ)[5], substitute $(\frac{Ze^2\psi}{r})$ instead of (eφ) we obtain:

$$E_k=\frac{12}{5}(\frac{2}{9\pi^2})^{1/3}Z^{7/2}\frac{me^4}{h^2}\int_0^\infty\psi^{3/2}\frac{dx}{\sqrt{x}}.....(12)$$

The potential energy is divided to two parts first the interaction between the electrons and nucleons.

$$E_{pot}^{[1]} = -\int_0^\infty \frac{Ze^2}{r} n4\pi r^2\, dr \ldots\ldots(13)$$

(n) can be defined from the equation (6).
Second the interaction between the electrons them selves:

$$E_{pot}^{[2]} = -\frac{1}{2}\int_0^\infty \frac{Ze^2}{r} n(1-4)\pi r^2\, dr \ldots\ldots(14)$$

The number (1/2) refers that the electron must be take in to account once.

$$E_{pot} = E_{pot}^{[1]} + E_{pot}^{[2]} = -1/2\int_0^\infty \frac{Ze^2}{r}(1+\psi) n4\pi r^2\, dr \ldots\ldots\ldots(\quad 15)$$

Substitute (n) we obtain:

$$E_{pot} = -2\left(\frac{2}{9\pi^2}\right)^{1/3} Z^{7/2}\frac{me^4}{h^2}\int(\psi^{7/2}+\psi^{5/2})\frac{dx}{\sqrt{x}} \ldots\ldots\ldots(16)$$

For the first integral use eq. (10):

$$\int_0^\infty \psi^{3/2}\frac{dx}{\sqrt{x}} = \int_0^\infty \psi''\, dx = \psi'(0) \ldots\ldots\ldots\ldots(17)$$

Because $\psi(\infty)$ should equals (zero).
For the second integral we can do it by part[6]:

$$\int_0^\infty \psi^{5/2}\frac{dx}{x} = 2\sqrt{x}\,\psi^{5/2}\Big|_0^\infty - 5\int_0^\infty \sqrt{x}\,\psi^{3/2}\psi' dx$$

$$= -5\int_0^\infty x\psi''\psi' dx = -\frac{5}{2}\int_0^\infty x\frac{d}{dx}(\psi')^2 dx$$

$$= -\frac{5}{2}x(\psi')^2\Big|_0^\infty + \frac{5}{2}\int_0^\infty (\psi')^2 dx \ldots\ldots\ldots\ldots\ldots(18)$$

But (ψ') approaches zero more rapidly than (1/x) when x→∞ so:

$$\int_0^\infty (\psi')^2 dx = \psi\psi'\Big|_0^\infty - \int_0^\infty \psi\psi' dx = -\psi'(0) - \int_0^\infty \psi^{5/2}\frac{dx}{\sqrt{x}} \ldots\ldots\ldots(19)$$

$$\int_0^\infty \psi^{5/2}\frac{dx}{\sqrt{x}} = \frac{5}{2}\left[-\psi'(0) - \int_0^\infty \psi^{5/2}\frac{dx}{\sqrt{x}}\right]$$

$$\int_0^\infty \psi^{5/2}\frac{dx}{\sqrt{x}} = -\frac{5}{2}\psi'(0).....(20)$$

Substitute the values of the integrals in E_k and E_{pot} we obtain: $E_{pot} = -2E_k$ and total energy $E = -E_k$

$\psi'(0)$ can be found from the equation ($\varphi = \frac{Ze^2\psi}{r}$) and from the ionization voltage for Hydrogen atom $\Psi^1(0) = -1.589$. therefore we obtain the equation:

$$E = -0.769\frac{me^4}{h^2}Z^{7/3} = 0.769\frac{9.107\times10^{-28}\times(4.8\times10^{-18})^4}{(1.03\times10^{-34})^2}Z^{7/3}$$
$$= 33.504\times10^{-19}Z^{7/3}Joul$$
$$= 20.94Z^{7/3}ev$$
$$= 0.76703Z^{7/3}AU$$

***Elements* (Z)**	***H.F. in (AU)***	***E_0 (AU)***	***$E(H.F)/E_0$ %***
Ae (2)	*2.862*	*3.870*	*73.95*
Li (3)	*7.4320*	*09.9680*	*74.55*
Be (4)	*14.573*	*019.500*	*74.71*
B (5)	*24.529*	*032.830*	*74.73*
C (6)	*37.688*	*044.350*	*75.10*
N (7)	*54.400*	*071.900*	*75.60*
O (8)	*74.809*	*098.300*	*76.09*
F (9)	*99.409*	*129.390*	*76.80*
Ne (10)	*128.597*	*165.460*	*77.70*
Na (11)	*161.858*	*206.670*	*78.30*
Mg (12)	*199.614*	*253.190*	*78.80*
P (15)	*340.718*	*426.160*	*79.92*
Ca (20)	*676.758*	*833.860*	*81.10*
Mn (25)	*1199.866*	*1403.53*	*81.70*
Zn (30)	*1777.848*	*2197.70*	*83.01*
Br (35)	*2572.441*	*3149.50*	*84.50*
Zr (40)	*3539.995*	*4202.40*	*84.60*
Rh (45)	*4685.881*	*5531.60*	*84.70*
Sn (50)	*6022.931*	*7073.30*	*85.10*
Xe (54)	*7232.138*	*8464.70*	*85.40*

Table (1): Hartree- Fock total energies and a compassion with their values from the equation (21).

***Elements* (Z)**	E_i ***in (AU)***	E_0 ***(AU)***	E_i / E_0 ***%***
Lu (70)	*14992.31*	*15509.2*	*96.60*
Re (75)	*1788200*	*18218.14*	*98.12*
Hg (80)	*20973.3*	*21178.90*	*99.03*
At (85)	*24270.2*	*24397.30*	*99.47*
Th (90)	*27850.21*	*27877.90*	*99.90*
U (92)	*36668.7*	*30032.60*	*99.92*

Table (2): E_i is international values of Binding energies for heavy element obtain from laser technology Masashusits institute, E is the binding energy obtain from equation (21) in the research.

Conclusion:

Its evident from the results in tables (1,2) that the binding energy for electron increase as the atomic number (Z) increase. As if as we said in the research that the binding energy composed of two parts positive energy because the interaction between the electrons them selves and negative energy because the interaction of electrons with nucleus.

In fact whenever the atomic number increase the electron approaches to the nucleus that is the probability for electron to become more near to the nucleus but the approaching of electrons to each other become less for the inner electrons decrease the effect of the charge of nucleus.

We see from the two tables that the agreement of the values of binding energy obtained from eq.(21) with that internationally accepted become more precisely as the atomic number increase that is because eq.(21) is derived statistically and statistic is more precise when the particles in the problem become more.

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