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Quantum Electro-dynamic Corrections of $1s_{1/2}$ Energy Level in Hydrogen like Atoms

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Abstract: *We have calculated the one loop QED corrections in $1s_{1/2}$ level for hydrogen like atoms for Z=1-92. The self energy (which now automatically contains the vertex correction) and the vacuum polarization corrections are calculated with finite size nucleus. The results are calculated using non relativistic and relativistic approaches. For light nuclei (Z=1-20) the two approaches give approximately the same results. For heavy nuclei (Z=20-92) the relativistic effect increases with increasing Z. The effect of finite size on the low energy part of self energy and the total energy shift is very small for light atoms and increases slowly with Z until Z=20 and begins to decrease until Z=80 and then increases for higher Z. The volume of the nucleus gives a large difference for high Z in the vacuum polarization and increases the vertex correction slowly with Z. The contribution of the shape of the density of light nuclei is very small.*
Keywords*: Self energy, vacuum polarization and vertex corrections; Point nucleus; Finite size nucleus; Hydrogen like atoms; $1s_{1/2}$ energy level.*

I. Introduction

The vacuum fluctuations predicted by QED are clear in their influence on the energy of bound states in atoms. Since atomic transition energies are measured by spectroscopic methods very accurately, the calculation of level shifts gives a good test for the validity of the theory. This problem is very difficult. Besides we are dealing with bound states which can interact with the charge Ze of the nucleus any number of times. Therefore one has to use the Dirac Coulomb wave functions. Mohr [1, 2] calculated the one photon self energy radiative $1s_{1/2}$ level shift of an electron in a Coulomb field for hydrogen like atoms. Soff and Mohr [3] examined vacuum polarization in a strong external field. Jentchura et al [4] evaluated the one-photon electron self energy for the k- and L-shell states of hydrogen like ions with nuclear charge numbers Z=1 to 5. El-Shabshiry et al [5] calculated the finite size effect of the nucleus on the energy levels of hydrogen atom.

In this work we have concerned with the evaluation of the finite size effect on the $1s_{1/2}$ bound state level shift associated with the self energy, vertex correction and vacuum polarization for hydrogen like atoms of Z in the range 1- 92.

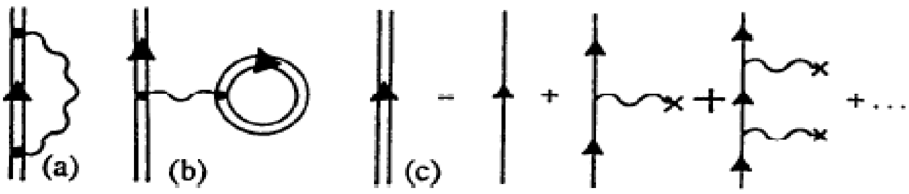


Fig.1. Graphs for
(a) self energy (b) vacuum polarization (c) Interacting electron propagator

II. One Photon Exchange QED Corrections

To evaluate QED corrections, one finds that light atoms $(Z\alpha) << 1$ allow for an approximate method of high accuracy. This method depends on the fact that the atomic binding energies are of the order of magnitude of $(Z\alpha)^2 m$ and hence electron states in light atoms can be treated non-relativstically. Thus one can split the evaluation of self energy into two steps 1) If the virtual emitted photon is of high energy $\omega \geq K >> (Z\alpha)^2 m$, the effect of Coulomb potential can be neglected and one may use free states for calculation. 2) If the virtual emitted photon is of low energy $\omega \leq K << m$ then one can use ordinary quantum mechanical perturbation theory for the Schrodinger equation.

This procedure work successfully when one chooses the separating energy K satisfies $m >> K >> (Z\alpha)^2 m$ (1)

in light atoms there is no problem. Adding the energy shifts obtained in two regions gives results independent on K.

The High Energy Part of Self Energy (Vertex Correction):

To calculate this part we use the form factors $\mathrm{F}_1(\mathrm{q}^2), \mathrm{F}_2(\mathrm{q}^2)$ for Free states.

$$\mathrm{F}_1(q^2) \approx \frac{\alpha}{3\pi}\frac{q^2}{m^2}(\ln\frac{m}{\mu}-\frac{3}{8}), \qquad \mathrm{F}_2(0) \approx \frac{\alpha}{2\pi}$$

In first order perturbation theory this high energy shifts takes the form:

$$\delta E^{high} = e\int d^3x\psi_\nu^+(x)[\frac{\alpha}{3\pi m^2}(\ln\frac{m}{\mu}-\frac{3}{8}-\frac{1}{5})\Delta\mathrm{A}^0(x)+\frac{\alpha}{2\pi}\frac{i}{2m}\vec{\gamma}\bullet\vec{E}]\psi_\nu(x) \tag{2}$$

Where,

$$\mathrm{A}^0(x) = \frac{-Ze}{|x|}, \tag{3}$$

is the Coulomb potential of the nucleus. K is the cut off parameter which play the role of $\Delta\mathrm{E}$ which is the energy below which no photons are observed. Then, in equation (2) one must replace

$$\ln\frac{m}{\mu} \to \ln\frac{m}{2K}+\frac{5}{6} \tag{4}$$

The energy shift can be written as

$$\delta\mathrm{E}_\nu = \delta E_\nu^{(1)} + \delta E_\nu^{(2)}$$

Where

$$\delta E_\nu^{(1)} = \frac{e\alpha}{3\pi m^2}(\ln\frac{m}{2K}+\frac{5}{6}-\frac{3}{8}-\frac{1}{5})\langle\nu|\nabla^2\mathrm{A}^0|\nu\rangle \tag{6}$$

and

$$\delta E_\nu^{(2)} = \frac{e\alpha}{8\pi m^2}[\langle\nu|\nabla^2\mathrm{A}^0|\nu\rangle + 4\langle\nu|\frac{1}{r}\frac{d\mathrm{A}^0}{dr}\vec{S}\bullet\vec{L}|\nu\rangle] \tag{7}$$

The Contribution of Low energy Emitted Photons:

The unperturbed problem is described by the Schrodinger eq.

$$\hat{\mathrm{H}}_o\psi_\nu = (-\frac{\nabla^2}{2m}+e\mathrm{A}^0(x))\psi_\nu = E\psi_\nu \tag{8}$$

The perturbation operator

$$\mathrm{H}' = 2\frac{ie}{2m}\vec{\mathrm{A}}\bullet\nabla, \tag{9}$$

where $\vec{\mathrm{A}}$ is the potential of the transverse field. Since H' creates and annihilates photons, the energy shift in second order perturbation theory has the form

$$\delta E_{\nu}^{low\,\mathrm{energy}} = \sum_{\nu' k \lambda} \frac{|\langle \nu', k, \lambda | H' | \nu \rangle|^2}{E_{\nu} - (E_{\nu'} + \omega)} \tag{10}$$

ν' is the electron state, k is its momentum and λ is the polarization of the transverse field.

$$(\delta E_{\nu}^{low})_{ren} = \frac{e\alpha}{3\pi m^2}[\langle \nu | \nabla^2 \mathrm{A}^o | \nu \rangle + [\ln \frac{2K}{m} - 2\ln(Z\alpha)]$$
$$+ \frac{2\alpha}{3\pi}\sum_{\nu'} |\langle \nu' | \mathrm{v} | \nu \rangle|^2 (E_{\nu'} - E_{\nu}) \ln \frac{(Z\alpha)^2 (m/2)}{|E_{\nu'} - E_{\nu}|} \tag{11}$$

The Total Energy Shift

It is given by the following equation:

$$\delta E_{\nu} = \frac{e\alpha}{3\pi m^2}(\frac{5}{6} - \frac{1}{5} - 2\ln(Z\alpha))\langle \nu | \nabla^2 \mathrm{A}^0 | \nu \rangle + \frac{e\alpha}{2\pi m^2}\langle \nu | \frac{1}{r}\frac{d\mathrm{A}^0}{dr} \vec{S} \bullet \vec{L} | \nu \rangle$$
$$+ \frac{2\alpha}{3\pi}\sum_{\nu'} |\langle \nu' | \mathrm{v} | \nu \rangle|^2 (E_{\nu'} - E_{\nu}) \ln \frac{(Z\alpha)^2 (m/2)}{|E_{\nu'} - E_{\nu}|} \tag{12}$$

For point charge nucleus

$$\delta E_{n\ell j} = \frac{4m}{3\pi n^3}\alpha (Z\alpha)^4 \{L_{n,\ell} + [\frac{19}{30} - 2\ln(Z\alpha)]\delta_{\ell 0} \pm \frac{3}{4}\frac{1}{(2j+1)(2\ell+1)}(1 - \delta_{\ell 0})\} \tag{13}$$

for states with $j = \ell \pm \frac{1}{2}$. Where $L_{n\ell}$ is the *Bethe logarithm*

$$L_{n\ell} = \frac{n^3}{2m(Z\alpha)^4}\sum_{\nu'} |\langle \nu' | \mathrm{v} | \nu \rangle|^2 (E_{\nu'} - E_{\nu}) \ln \frac{(Z\alpha)^2 (m/2)}{|E_{\nu'} - E_{\nu}|}$$

In this work we tried to find the finite size effect on the $1s_{1/2}$ level of hydrogen-like atoms for Z=1-92. We divide the range of energy emitted by the photon in self energy into:

a) High energy part in this case we calculate the finite size contributions to the vertex correction by taking free form factors and substituting about the separating energy (K = *m*) as Bethe. From equation (6)

$$\delta E_{ver}^{high} = \frac{e\alpha}{3\pi m^2}(\ln(\frac{1}{2}) + \frac{5}{6})\langle \nu | \nabla^2 \mathrm{A}^0 | \nu \rangle \tag{14}$$

b) Low energy part from eq. (11)

$$\delta E_{self}^{low} = \frac{e\alpha}{3\pi m^2}[\langle \nu | \nabla^2 \mathrm{A}^0 | \nu \rangle [\ln(2) - 2\ln(Z\alpha)] + \frac{4\alpha (Z\alpha)^4 m}{3\pi} L_{n\ell} \tag{15}$$

and the correction due to vacuum polarization from the formula

$$\delta E_{vac} = -(\frac{1}{5}\frac{e\alpha}{3\pi m^2}\langle \nu | \nabla^2 \mathrm{A}^o | \nu \rangle) \tag{16}$$

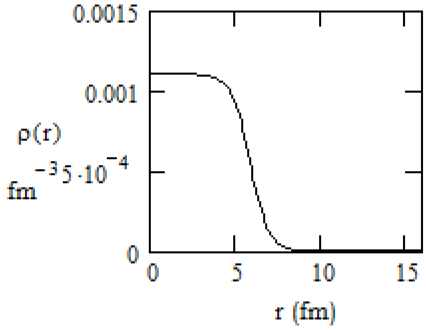


Fig. 2: The Fermi charge density of the nucleus (Z=92) against r.

Substituting about

$$\frac{e\alpha}{3\pi m^2}\langle v|\nabla^2 \mathrm{A}^o|v\rangle = \frac{4\pi Z\alpha^2}{3\pi m^2}\int \rho(r)|\psi_{n\ell}|^2 r^2 dr \tag{17}$$

in equations (14), (15) and (16) we obtain the corresponding formulas for finite size nucleus, where $\rho(r) = \dfrac{\rho_o}{1+e^{(r-R)/D}}$ is the density of the nucleus, $\psi_{n\ell}$ is the $1s_{1/2}$ wave function of the electron which is taken one time non-relativistic and one time as Dirac wave function of electron in a Coulomb field, to show the relativistic effect.

Table 1: Represents the comparison between the corrections calculated for point and finite size nucleus.

Z	δE^{point}_{vac} **(eV)**	δE^{Sch}_{vac} **(eV)**	δE^{point}_{ver} **(eV)**	δE^{Sch}_{ver} **(eV)**	δE^{point}_{self} **(eV)**	δE^{Sch}_{self} **(eV)**
1	-8.976×10^{-7}	-9.034×10^{-7}	6.291×10^{-7}	6.332×10^{-7}	6.067×10^{-5}	6.097×10^{-5}
2	-1.436×10^{-5}	-1.309×10^{-5}	1.007×10^{-5}	9.178×10^{-6}	9.127×10^{-4}	9.525×10^{-4}
3	-7.27×10^{-5}	-6.459×10^{-5}	5.096×10^{-5}	4.528×10^{-5}	0.00491	0.00475
5	-5.61×10^{-4}	-4.747×10^{-4}	3.932×10^{-4}	3.327×10^{-4}	0.01279	0.00963
10	-0.00898	-0.00726	0.00629	0.00509	0.1373	0.08645
15	-0.04544	-0.03277	0.03185	0.02297	0.5929	0.2688
20	-0.1436	-0.09079	0.1007	0.06364	1.766	0.5666
30	-0.727	-0.3475	0.5096	0.2436	7.306	0.225
40	-2.298	-0.8213	1.611	0.5757	19.21	-4.085
50	-5.61	-1.461	3.932	1.024	41.65	-14.57
60	-11.63	-2.203	8.154	1.544	79.82	-30.74
70	-21.55	-2.885	15.11	2.022	127.7	-62.41
80	-36.76	-3.567	25.77	2.499	217.8	-75.95
90	-58.89	-4.067	41.28	2.851	415.1	-5.373
92	-64.3	-4.126	45.07	2.893	473.3	24.97

Table 2: Represents the total energy shift. The second column for point charge, the third for non-relativistic finite size nucleus and the fourth for vacuum polarization and the vertex calculated with finite size + self energy for point charge nucleus.

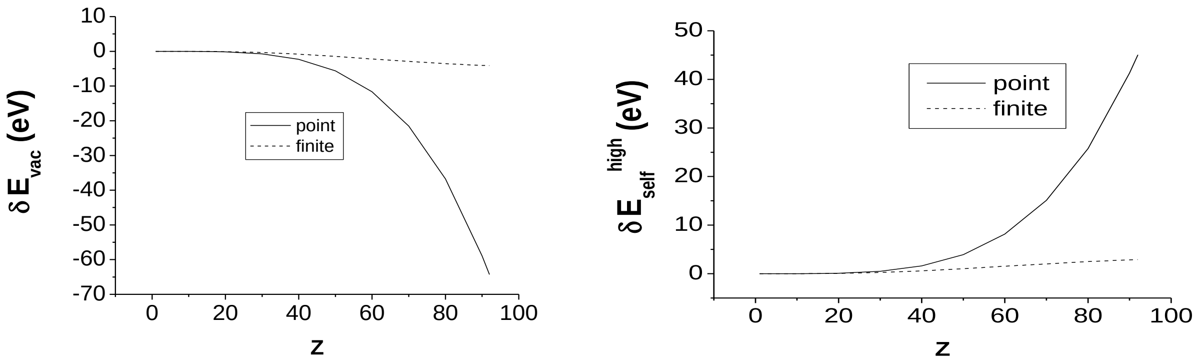
Z	δE^{point} **(eV)**	δE^{finite}_{Sch} **(eV)**	$[\delta E^{Sch(finite)}_{vac} + \delta E^{Sch(finite)}_{ver} + \delta E^{Sch(point)}_{self}]$ **(eV)**
1	6.04015×10^{-5}	6.06998×10^{-5}	6.03998×10^{-5}
2	9.0841×10^{-4}	9.48588×10^{-4}	9.08788×10^{-4}
3	0.00489	0.00473	0.00489
5	0.01262	0.00949	0.01265
10	0.13461	0.08428	0.13513
15	0.57931	0.259	0.5831
20	1.7231	0.53945	1.73885
30	7.0886	0.1211	7.2021
40	18.523	-4.3306	18.9644
50	39.972	-15.007	41.213
60	76.344	-31.399	79.161
70	121.26	-63.273	126.837
80	206.81	-77.018	216.732
90	397.49	-6.589	413.884
92	454.07	23.737	472.067

Table 3: Represents the comparison between the non- relativistic and relativistic total energy shift in the $1s_{1/2}$ level calculated for finite size nucleus.

Z	δE^{finite}_{Sch} (eV)	$\delta E^{finite}_{Dirac}$ (eV)
1	6.06998 x10^{-5}	5.98447 x10^{-5}
2	9.48588 x10^{-4}	9.48319 x10^{-4}
3	0.00473	0.00469
5	0.00949	0.01059
10	0.08428	0.08722
15	0.259	0.28054
20	0.53945	0.61988
30	0.1211	0.5519
40	-4.3306	-3.1348
50	-15.007	-12.796
60	-31.399	-28.183
70	-63.273	-59.555
80	-77.018	-73.113
90	-6.589	-3.087
92	23.737	27.075

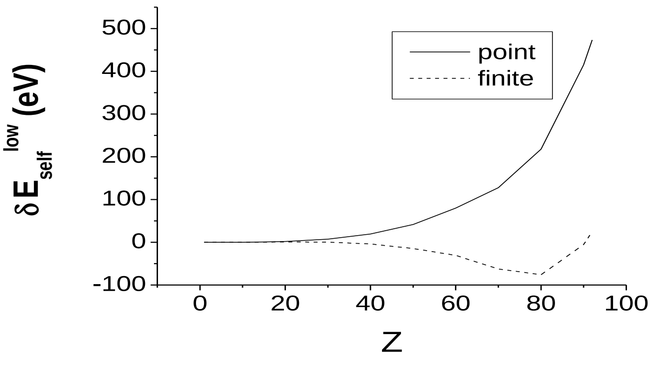
III. Results and Discussion

In this paper the natural units are used $\hbar = c = 1$. The density of the nucleus is taken as Fermi distribution, the r.m.s radius of different nuclei is taken from Brown et al [6]. Figure (2) represents the Fermi charge density of the nucleus (Z=92). Figure (3) consists of a, b and c. It shows the variation of the QED corrections calculated non-relativistically for point and finite size nucleus with Z.



(a) vacuum polarization

(b) vertex [high energy part of self energy] correction



(c) self energy [low energy part]

Fig. (3): Represents the comparison between the above three corrections calculated with and without finite size of the nucleus in non-relativistic case.

For light atoms (Z=1-20) the finite size effect is very small and then increases slowly for higher Z nuclei. The difference between the point charge and finite size results is very clear for higher Z nuclei. In figure (4) the effect of finite size on the total energy shift is very clear for heavy atoms.

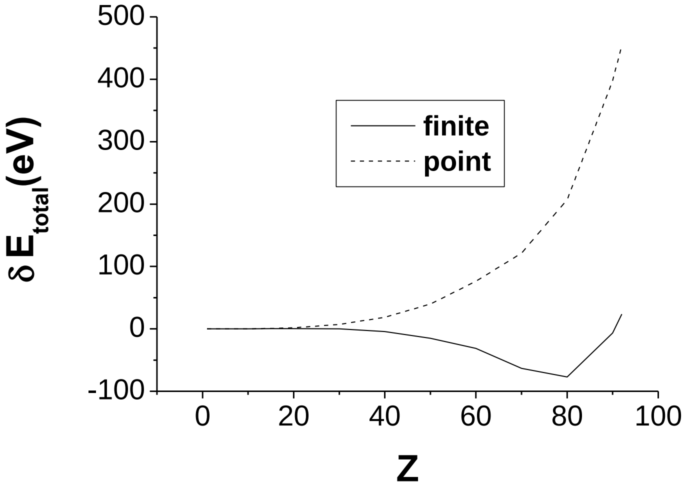


Fig. (4) Represents the variation of the total energy shift calculated non-relativistically with and without finite size charge of the nucleus.

In figure (5) the low energy part of self energy is calculated for point charge nucleus and added to the vacuum polarization and vertex correction calculated for finite size nucleus, in this case the total energy shift gives reasonable agreement with the experimental data [7].

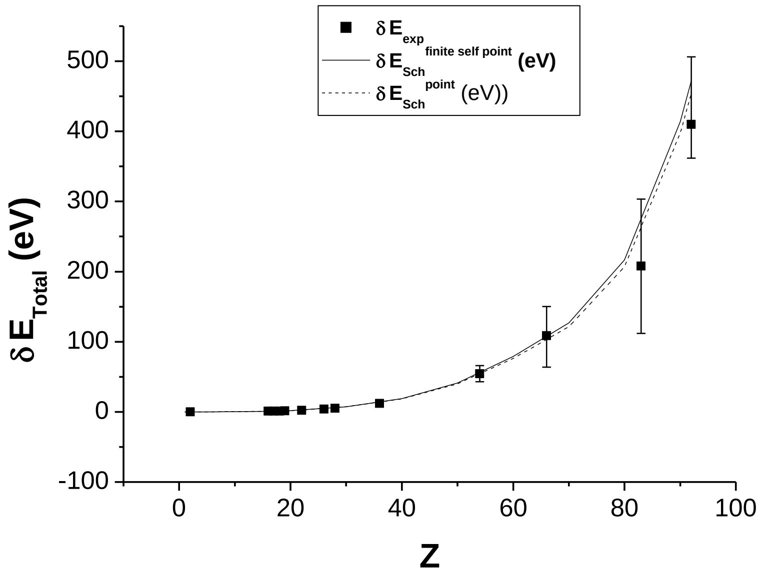
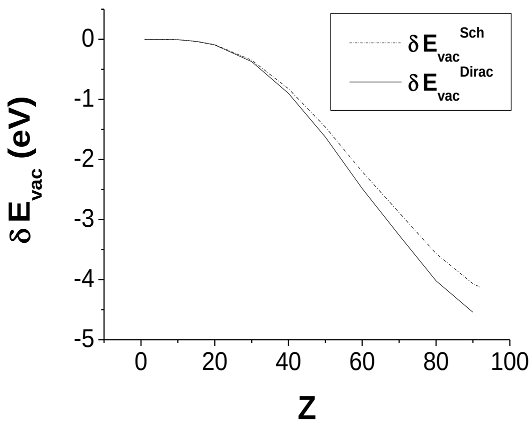
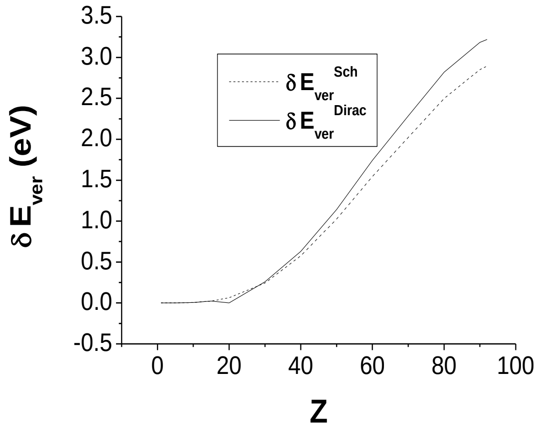


Fig. (5): Same as figure (4) with the low energy part of the self energy calculated for point charge nucleus.

Figure (6) the relativistic and non-relativistic values of the total energy correction calculated for finite size nuclei



(a)



(b)

Fig. 6: The relativistic effect for a) vacuum polarization (b) Vertex correction.

Figure (7) represents the relativistic and non-relativistic values of the total energy correction calculated for finite size nuclei.

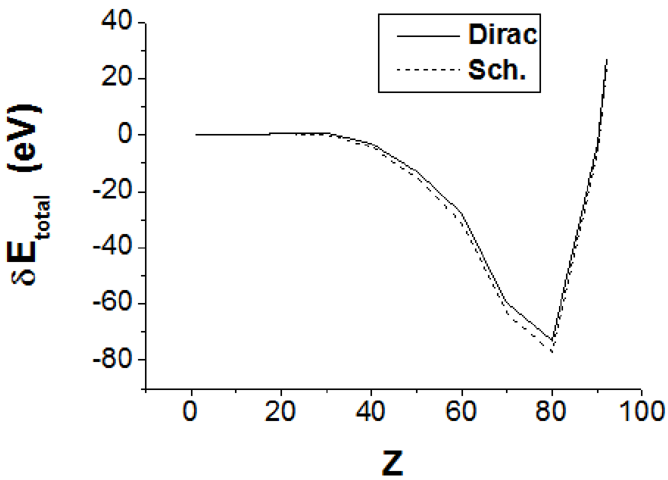


Fig. (7): Represents the variation of the total energy shift of the $1s_{1/2}$ level for finite size nucleus with Z, calculated in case of Dirac w. f. and in case of Schrödinger w.f.

The correction is constant for light nuclei it decreases smoothly with Z until Z=80 and increases fastly for higher Z nuclei. The difference between relativistic and non- relativistic values is small. From figure (8), the shape of the nucleus density has a very small contribution to the total correction for light atoms.

Table 4: Shows the non-relativistic and relativistic results of the total energy shifts in the $1s_{1/2}$ level for light hydrogen like atoms (Z= 1-15). The calculations are performed by using Fermi and Gaussian distributions for the light nucleus density.

Z	δE_{Sch}^{finite} **(eV)**	δEG_{Sch}^{finite} **(eV)**	$\delta E_{Dirac}^{finite}$ **(eV)**	$\delta EG_{Dirac}^{finite}$ **(eV)**
1	6.06998×10^{-5}	6.011×10^{-5}	5.98447×10^{-5}	6.013×10^{-5}
2	9.48588×10^{-4}	9.516×10^{-4}	9.48319×10^{-4}	9.522×10^{-4}
3	0.00473	0.00474	0.00469	0.004746
5	0.00949	0.011	0.01059	0.01109
10	0.08428	0.08607	0.08722	0.08911
15	0.259	0.2.654	0.28054	0.2878
20	0.53945	0.5393	0.61988	0.6217

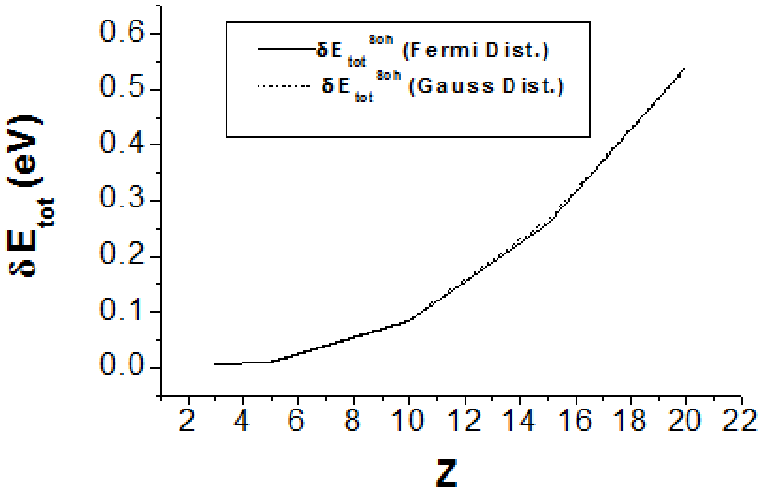


Fig. 8: The non-relativistic Total energy correction against Z in case of Fermi and Gaussian density for light nucleus atoms.

Finally one can conclude that the effect of finite size of the nucleus on the shift in $1s_{1/2}$ level is very small for light atoms (Z=1-20). The size effect on the low energy part of self energy is higher than on the vacuum polarization and vertex corrections for heavy atoms (table 2). The difference between the corrections calculated relativistically and non-relativistically is small. To show the effect of the form density of the nucleus, we calculate the total energy correction in case of Gaussian and Fermi forms.

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