CHAPTER 4

RESULTS AND DISCUSSION

4.1. EXCHANGE COULOMB ENERGY AS A FUNCTION OF MASS NUMBER

4.1.1. Closed shell nuclei

Calculations using exact expressions for the Coulomb interaction were first performed for a series of closed and doubly closed shell (spherical) nuclei ranging from light to super heavy ones. As the exact Coulomb treatment (as opposed to a Slater approximation) affects only the exchange part, the main result of the present study consists in the magnitude of the exchange Coulomb energy difference. The difference in exchange Coulomb energy is presented in terms of percentage defined by:

$$(\%)_{diff\_exact\_coul} = \frac{E_{exact} - E_{Slater}}{E_{exact}} \times 100$$

where E_{exact} refers to the exact calculation of the exchange Coulomb energy while E_{Slater} is the exchange Coulomb energy calculated using the Slater approximation.

Figure 4.1 shows the percentage difference (error) in the exchange Coulomb energy for magic nuclei calculated using the SkM* interaction. Pairing interaction is known to be unimportant for nucleon numbers in a given charge state which are magic. One can thus neglect it for doubly magic nuclei. From Figure 4.1, it is apparent that the percentage error decreases, as expected, with increasing mass number, A. One observes

that for Oxygen-16, the difference in exchange Coulomb energy is close to 8 % compared to Calcium-40 which is about 5 %. Nuclei with mass number around 100 and above exhibit a slower decline of the percentage energy difference as a function of A, in the region of 2-4 %. As we have already discussed, the declining pattern of the correction in exchange Coulomb energy with increasing mass number can be attributed to the plane wave assumption used in the Slater approximation. This assumption is of course less suitable for light nuclei since they are much too small in size to present a significant saturated density region and their wavefunctions cannot be described properly by plane waves. On the other hand, we know that with increasing mass number, the radius of the nucleus increases as well with the saturation relation:

$$R = r_0 A^{1/3}$$

Therefore, heavy nuclei have a larger extension of radius making it more reasonable to approximate the single particle wavefunctions as plane waves.

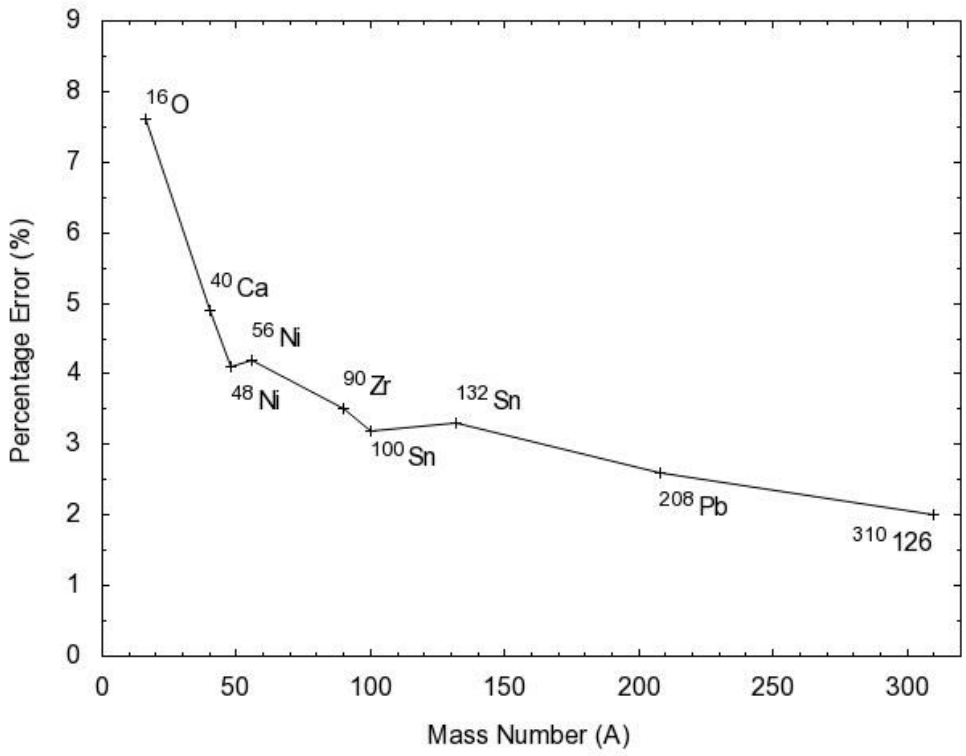

Figure 4.1: Difference in exchange Coulomb energy given in percentage calculated using SkM* force for closed and semi-closed nuclei

The percentage exchange Coulomb energy obtained by Skalski (2001) calculated using the SkP parameterization are presented in Figure 4.2 as individual points along our present results obtained using SkM* for comparison. The agreement between the two results is indeed very striking which has led Skalski in his work to conclude that the results are interaction independent. To support further this idea, calculations were made for the three lighter closed shell nuclei using the SIII force which had been used in the pioneering work of Titin-Schnaider and Quentin (1974) for some light nuclei with a much smaller basis size. Our results are compared in Table 4.1 with theirs. They are very close. Table 4.2 gives the percentage exchange Coulomb energy difference from the present calculation and those of Skalski using the SkP force. They are very much in agreement. One could thus confirm the conclusion that indeed the results do not depend on the type of nucleon-nucleon force used in the calculation (provided of course that they are reasonably realistic).

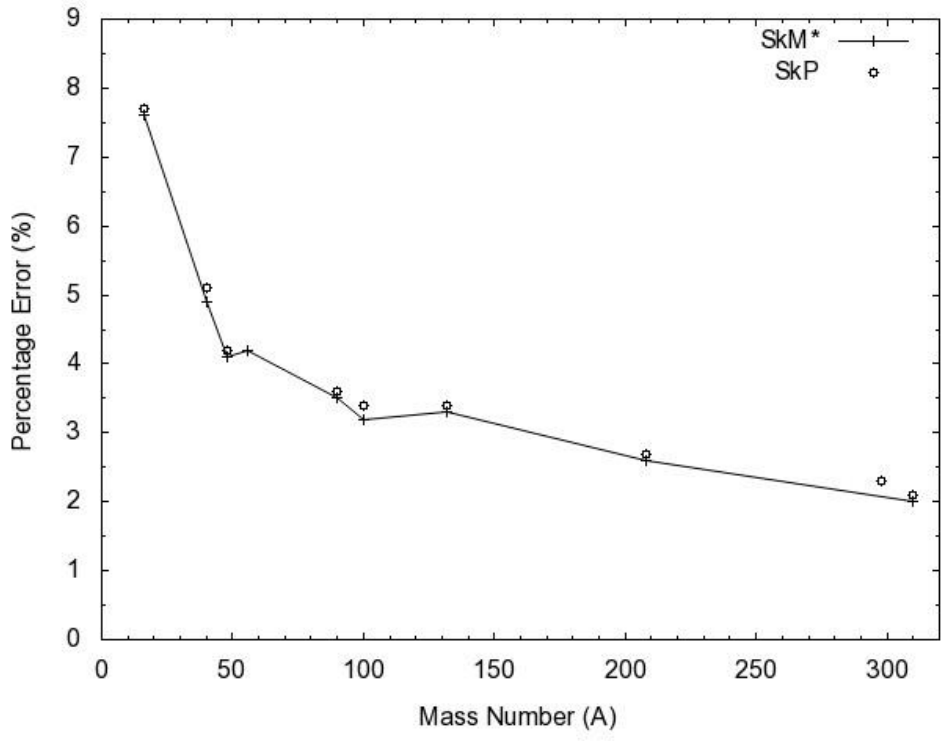

Figure 4.2: Comparison of percentage exchange Coulomb energy difference using SkP and SkM* forces.

Table 4.1: Results of the exchange Coulomb energy (in MeV) from exact calculation and the difference in the exchange Coulomb energy (in percentage). The last two columns correspond to the results obtained from T. Schnaider and Quentin (1974) using SIII force.

	A	**This work**		**Titin-Schnaider & Quentin (1974)**	
		$E_{exact\_exch\_coul}$	**%**	**$E_{exact\_exch\_coul}$**	**%**
O	16	-3.106	7.6	-3.110	7.7
Ca	40	-7.918	4.9	-7.910	4.9
Ni	56	-11.328	4.3	-11.230	4.4

Table 4.2: Exchange Coulomb energy given in MeV and the energy difference (in percentage) from present work and those of Skalski (2001).

Nucleus	**A**	**SkM* (this work)**		**SkP from Skalski (2001)**	
		$E_{exact\_exch\_coul}$	**%**	**$E_{exact\_exch\_coul}$**	**%**
O	16	-3.039	7.6	-3.009	7.7
Ca	40	-7.859	4.9	-7.826	5.1
Ni	48	-11.359	4.1	-11.258	4.2
Ni	56	-11.387	4.2	-	-
Zr	90	-15.875	3.5	-15.816	3.6
Sn	100	-20.476	3.2	-20.367	3.4
Sn	132	-19.508	3.3	-19.450	3.4
Pb	208	-32.117	2.6	-32.077	2.7
Z=114	298	-	-	-44.193	2.3
Z=126	310	-49.273	2.0	-49.249	2.1

4.1.2. Isotonic series

Having some inkling on the magnitude of the correction due to the Slater approximation for magic and semi-magic nuclei, it is then interesting to extend the study beyond the closed shells. Since the Coulomb interaction takes place between protons, it is imperative to investigate the trend of the correction due to the Slater approximation by varying the number of protons in the nucleus. Figure 4.3 shows the difference in exchange Coulomb energy for different isotonic series, calculated by constraining the nucleus to be of spherical shape. The nucleus that gives the largest correction for each series is labelled in the figure. The choice of the basis size and the pairing strength parameter (G_n for neutron and G_p for proton) used in the calculation of isotonic series depends on the mass number A, as given in Table 4.3. The top of the single particle energy window (above the Fermi level) used for the pairing calculations is also listed. It was set to 5.0 MeV with a diffuse cut-off of 0.2 MeV except for very heavy nuclei with mass numbers larger than 230 in which case a 6.0 MeV window was used.

Table 4.3: List of basis size, pairing window and pairing strengths for different mass number, A.

A	**N_0**	**Pairing window**	**Diffuseness**	**G_n (MeV)**	**G_p (MeV)**
< 100	10	5.0	0.2	17.1	16.5
< 130	12	5.0	0.2	17.1	16.5
< 208	12	5.0	0.2	18.0	17.5
> 230	14	6.0	0.2	14.3	15.5

One can clearly identify the nuclei that necessitate the largest correction for the exchange Coulomb energy. They are in fact doubly magic or magic nuclei. For example, ^{48}Ca and ^{56}Ni are doubly magic nuclei with atomic number and neutron

numbers 20 and 28, and 28 and 28 respectively. Moving away from magic numbers, the difference in the exchange Coulomb energy reduces dramatically as can be seen from the isotones N=78 series. Nevertheless, when the atomic number approaches a magic number the percentage difference increases again as shown in the isotones with N=106. The variation in the percentage difference as one moves away from a proton magic number is clearly shown in the two series of isotones with N=64 and N=126. Moreover, the percentage correction for magic nuclei is always larger than for non-magic nuclei. The magic nuclei included in this study dealing with some series of isotones, are ^{48}Ca, ^{56}Ni, ^{114}Sn and ^{208}Pb.

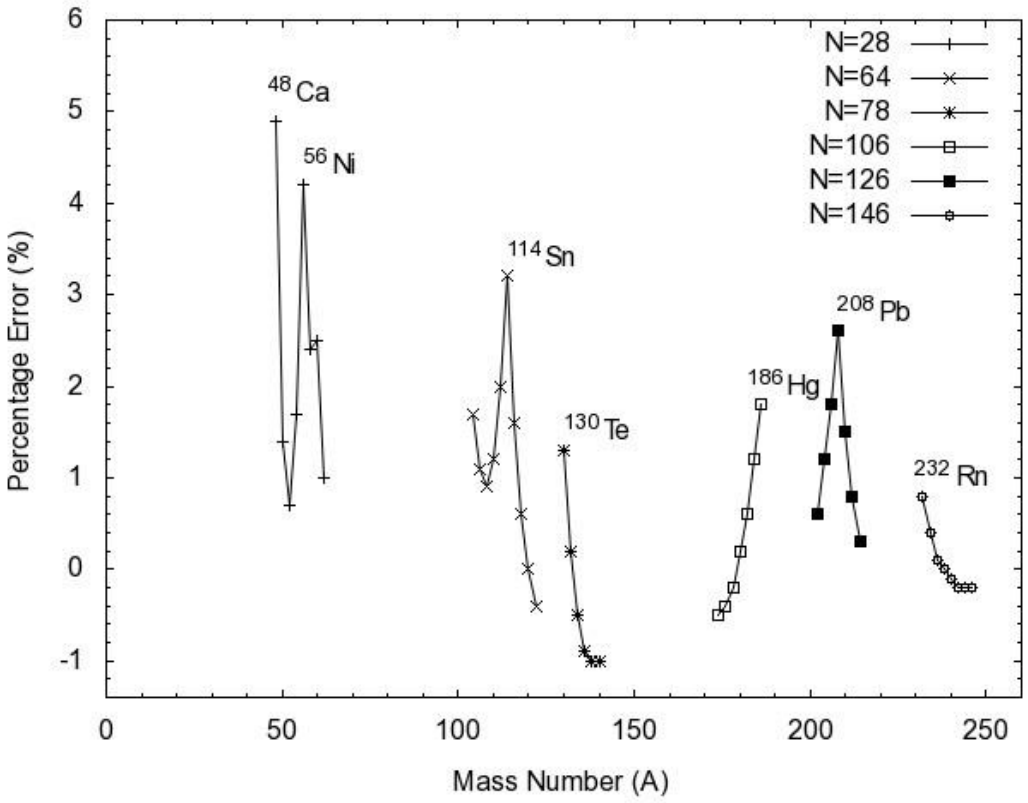

Figure 4.3: Difference in exchange Coulomb energy (given in %) for various isotones series.

From the results obtained from the study on magic nuclei, one would have expected that the percentage correction to the exchange Coulomb energy to decrease smoothly as a function of mass number. However, this is not the case as shown above

(see also Table 4.4 where these percentages are given along with the exact Coulomb energies). Away from magic number, one observes that the percentage correction is always smaller. The filling of the protons outside the closed shell into higher energy state does produce large variation in the percentage correction, an effect dubbed as a structural or shell effect.

4.1.3. Isotopic series

Finally, calculations were made for three isotopic series, namely for some Hafnium, Lead and Uranium isotopes to gain a more complete view of the percentage correction of the exchange Coulomb energy. We expect a priori the variation to be small since in all these series the proton number which has appeared important (in its closeness to a magic number) is invariant. The basis size and pairing parameters are as listed in Table 4.3. The calculation is also made upon imposing a spherical shape and the results are plotted in Figure 4.4 along with the previous results discussed earlier so as to give an overview on the subject matter. As it turns out, the variation of percentage correction for each individual isotopic series is rather small. Although the percentage correction increases with the number of neutrons, the increment is somewhat insignificant. Rather, one can conclude that the order of percentage correction for a particular isotopic series depends strongly on the distance of the atomic number from its neighbouring magic numbers. For example, the Hafnium and Uranium isotopes being non-magic nuclei have a very small percentage correction. In fact, the percentage corrections for these two isotopic series have negative values which mean that the Slater approximation overestimates the binding energy coming from the exchange part of the Coulomb interaction.

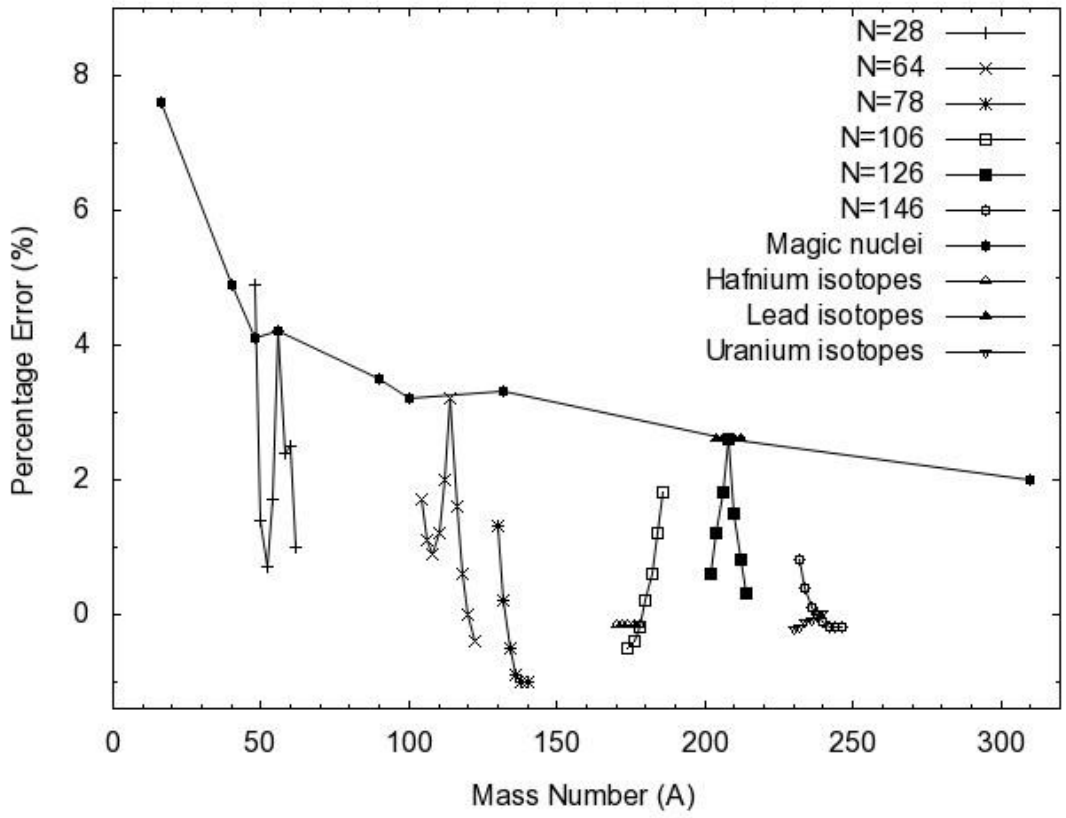

Figure 4.4: Results for all the calculations on magic nuclei, isotones and isotopes series with the nuclear shape constrained to be spherical.

On the other hand, isotopes of lead have a large correction of the exchange Coulomb energy because of the magic character of its atomic number. In this closed proton shell nuclei, the addition of neutrons into the nuclear system yields no effect whatsoever onto the percentage correction as shown in Figure 4.4.

To conclude this subsection 4.1, we may state that the correction of the exchange Coulomb depends almost completely only on the atomic number, Z, only, and in particular the distance of the atomic number away from magic numbers.

Table 4.4: Exchange Coulomb energy (in MeV) from exact calculation and percentage correction for isotonic series.

	Nucleus	**A**	**$E_{exact\_exch\_coul}$**	**%**
N=28	Ca	48	-7.811	4.9
	Ti	50	-8.391	1.4
	Cr	52	-9.198	0.7
	Fe	54	-10.190	1.7
	Ni	56	-11.388	4.2
	Zn	58	-11.965	2.4
	Ge	60	-12.771	2.5
	Se	62	-13.341	1.0
N=64	Zr	104	-15.165	1.7
	Mo	106	-15.954	1.1
	Ru	108	-16.800	0.9
	Pd	110	-17.752	1.2
	Cd	112	-18.812	2.0
	Sn	114	-19.994	3.2
	Te	116	-20.447	1.6
	Xe	118	-21.059	0.6
	Ba	120	-21.740	0.0
	Ce	122	-22.460	-0.4
N=78	Te	130	-20.012	1.3
	Xe	132	-20.612	0.2
	Ba	134	-21.299	-0.5
	Ce	136	-22.051	-0.9
	Nd	138	-22.858	-1.0
	Sm	140	-23.707	-1.0
N=106	Er	174	-25.534	-0.5
	Yb	176	-26.434	-0.4
	Hf	178	-27.368	-0.2
	W	180	-28.342	0.2
	Os	182	-29.360	0.6
	Pt	184	-30.423	1.2
	Hg	186	-31.528	1.8
N=126	Os	202	-28.805	0.6
	Pt	204	-29.861	1.2
	Hg	206	-30.957	1.8
	Pb	208	-32.117	2.6
	Po	210	-32.611	1.5
	Rn	212	-33.215	0.8
	Ra	214	-33.890	0.3
N=146	Rn	232	-32.509	0.8
	Ra	234	-33.209	0.4
	Th	236	-33.968	0.1
	U	238	-34.767	0.0
	Pu	240	-35.596	-0.1
	Cm	242	-36.436	-0.2
	Cf	244	-37.287	-0.2
	Fm	246	-38.152	-0.2

4.2. CORRECTION TO THE EXCHANGE COULOMB ENERGY AS A FUNCTION OF DEFORMATION

The viability of the Slater approximation as a function of deformation was tested on Selenium-70 (^{70}Se) for the quadrupole deformation mode. The pairing strength is chosen such that G_n = 17.1 MeV for neutrons and G_p = 16.5 MeV for protons. The pairing window is taken to be $[-\infty, \lambda + 5]$ in MeV (with λ being the chemical potential) with a diffuseness of 0.2 MeV (see subsection 3.6 for the definitions of these quantities).

The deformation energy curve of ^{70}Se (which was extensively studied in Bonneau and Quentin (2005)) was reproduced up to about 40 barn and it is plotted in Figure 4.5. The two points far on the right hand side of the figure corresponds to two ^{35}Cl separated fission fragments (note that we have obtained such a fragmentation since left-right reflection symmetry is assumed). At each of this point, an exact Coulomb calculation was made and the comparison of the exchange Coulomb energy (given in terms of percentage correction as defined above) was plotted in Figure 4.6.

At ground state (corresponding to a spherical shape), the Slater approximation is rather good giving rise to a small percentage error of about 0.6 %. However, the difference in exchange Coulomb between an exact calculation and the Slater approximation increases tremendously as the nucleus becomes more and more deformed. The percentage error peaks at about 4% at 15 barn before plummeting to about 2 % at 20 barn. Thereafter, the correction value remains range bound around 2.5 %. After the scission point (corresponding to the last two points on the far right in Figure 4.6), the percentage correction lies at about 2.2 %. These percentage corrections

together with the calculated values of the exact Coulomb exchange energy are reported in Table 4.5.

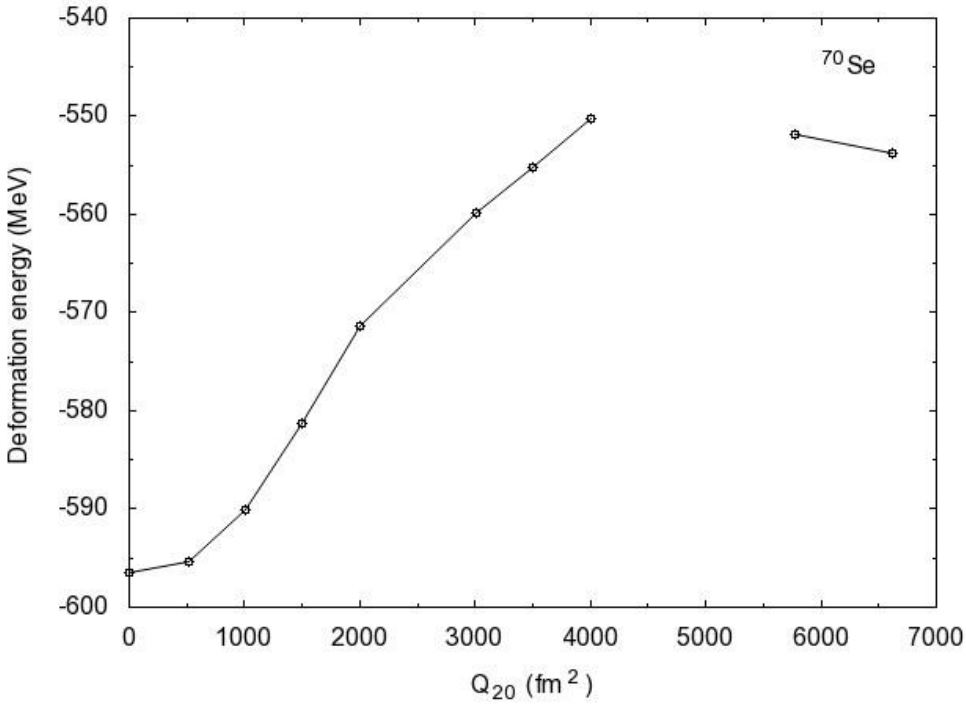

Figure 4.5: Deformation energy curve (in MeV) against quadrupole deformation (given in unit of fm^2) for ^{70}Se. The two disconnected points on the far right corresponds to the total energy of two fission fragments.

Leaving for the moment the two points where two different pieces of nuclear matter appear, we will now discuss some possible explanation for the behaviour of the percentage correction to the exchange Coulomb energy exhibited in Figure 4.6. Actually, we have found that a high value of the percentage error seems to be correlated with a low density of single particle proton energy levels at the Fermi sea surface (density which might have been obtained after Strutinsky averaged calculations or through a semi classical approximation).

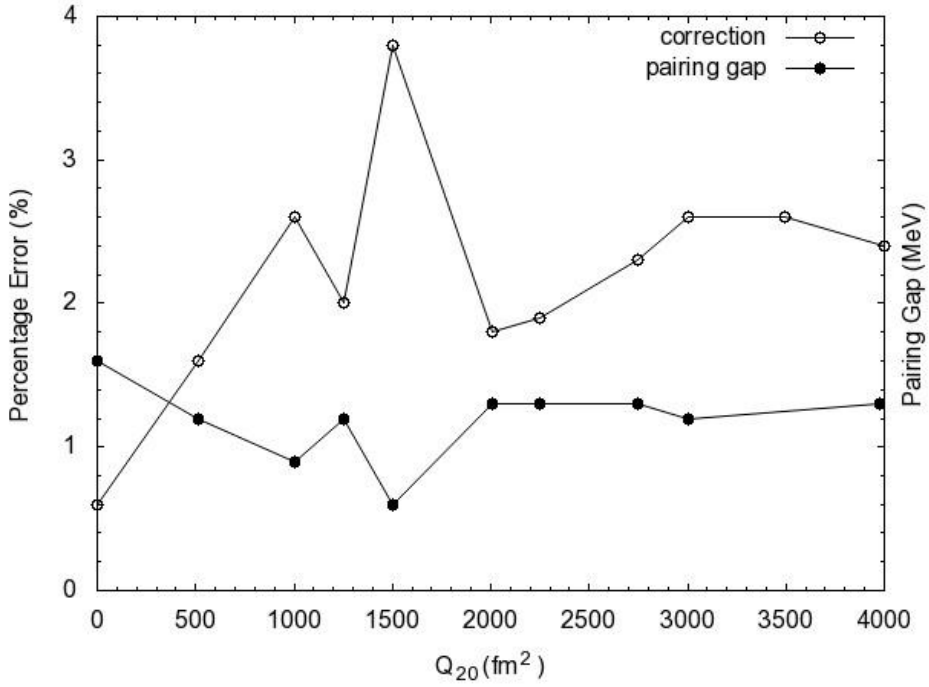

Figure 4.6: Correlation between proton pairing gap (in MeV) and the percentage correction at different quarupole deformation points for ^{70}Se.

This conclusion can only sketchily be drawn from the inspection of the proton single particle levels displayed on Figure 4.7. To be quantitative, we have considered as a relevant index for the level density, namely the proton pairing gaps. As can be seen from Figure 4.6 and Table 4.5, the variation with deformation of the gaps and the percentage corrections are very nicely correlated. This provides a strong support to our conjecture associating a high percentage correction with a low level density at the Fermi sea surface. The latter is also consistent with what has been obtained when varying Z. Varying the proton number or the deformation (at least in this range of deformation) the validity of the Slater approximation seems to be intimately correlated with the proton single particle level density near the Fermi energy. In effect, mid-shell nuclei correspond to a single particle level density much close to a semi-classically smoothed one and therefore one understands that the Slater approximation being of a (constant density) nuclear matter type, should be better in such cases than for low level density cases where the nuclear density is less close to its semi-classical approximation.

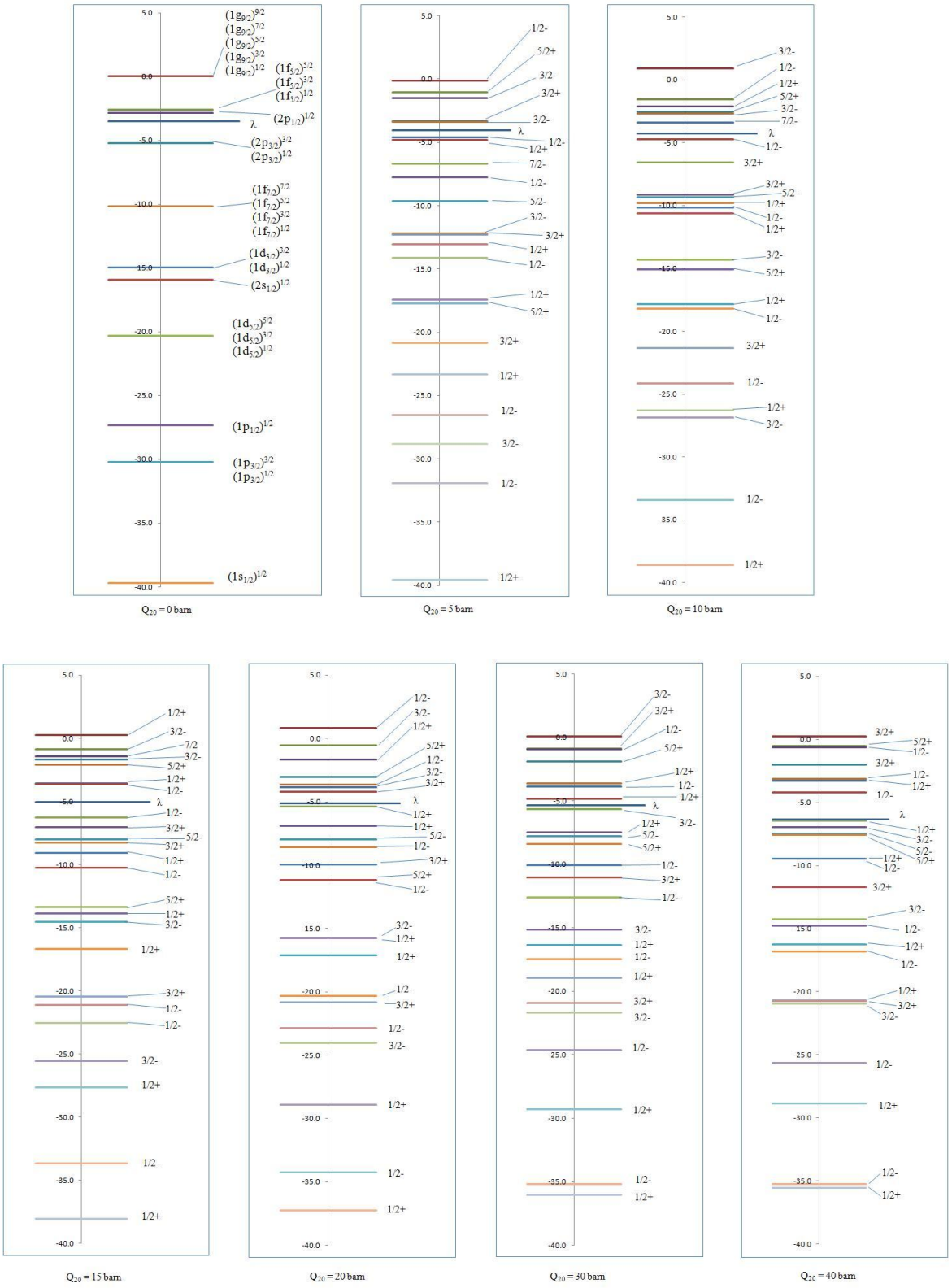

Figure 4.7: Proton single particle levels at different quadrupole deformations for ^{70}Se. The Fermi level is indicated in each of the spectrum by the symbol λ. The single particle level at 0 barn is labelled by its various quantum numbers $(nlj)^{\Omega}$ where n is the principal quantum number, l is the angular momentum, j is the total angular momentum with the relation $\boldsymbol{j = l \pm \frac{1}{2}}$ and Ω is the projection of j onto the z- axis with $\boldsymbol{\Omega = j, j - 1}$, ...

Table 4.5: Exchange Coulomb energy (in MeV) through exact calculation and the percentage correction to the Slater approximation at various quadrupole deformation points, Q_{20} (given in fm^2) for ^{70}Se.

Q_{20}	$E_{exact\_exch\_coul}$	%
0.0	-13.117	0.6
510.8	-13.323	1.6
1004.0	-13.332	2.6
1250.0	-13.182	2.0
1504.0	-13.411	3.8
2005.1	-13.031	1.8
2250.0	-13.038	1.9
2750.0	-13.060	2.3
3004.9	-13.089	2.6
3498.3	-13.039	2.6
3999.3	-12.935	2.4
5769.3	-12.896	2.2
6618.8	-12.897	2.2

CHAPTER 5

CONCLUSION

The present work aims at studying the Slater approximation to the exchange Coulomb energy in two a priori very different cases. The appropriateness of the Slater approximation was investigated on the one hand as a function of mass number while on the other hand, the effect brought upon by deformation of the nuclear shape was studied in a particular case.

In the first case, it was clearly shown upon studying spherical magic nuclei that the Slater approximation is more appropriate for heavy nuclei corresponding to large extension of the nuclear radius. For heavy nuclei, the correction to be brought to the Slater approximation is of the order of 2 % to 3 % as compared to light nuclei where it is for example in ^{16}O at about 8 %. This is expected since the Slater approximation, due to its intrinsic approximations, should perform well for larger size nucleus where a constant nuclear density approximation makes more sense. Indeed, in light nuclei almost all nucleon are in the density-varying surface region.

For open shell nuclei, the Slater approximation seems to be a much better approximation. The presence of nucleons (more specifically protons and not neutrons) outside the closed shells, an effect called the shell effect, seems to play a major role in lowering the order of correction to the Slater approximation.

This is confirmed by the study of the considered error as a function of the deformation in the ^{70}Se case. When changing the deformation, one explores different regimes of proton single particle (smoothed) level densities at the Fermi sea surface. It has been clearly established on one particular case that this level density and the percentage correction experience variations are anti-correlated. At a deformation where the level density is low the error on the Coulomb exchange energy is high as it is the case for a closed shell nucleus. When the former is high the latter is low as it is the case for a mid shell nucleus.

It seems therefore that we have exhibited a somewhat robust criterion to evaluate a priori the qualitative trend of the error made on the Coulomb exchange energy when varying the mean field either with some discrete parameter (as the proton number) or some continuous one (as a deformation parameter). This may allow one to hint the consequence of using, as usually made, the Slater approximation when evaluating a fission barrier height (e.g. the first fission barrier of a heavy nucleus). Clearly at the nuclear ground state, the value of the level density is smaller than its value at the top of the first fission barrier. Using the Slater approximation should thus lead to an underestimation of such a barrier. In actinide nuclei one may estimate that the error associated with a difference of 1% (in the percentage correction) between the ground state and the top of the barrier corresponds to an underestimation of the first barrier by about 0.35 MeV. This was verified for ^{238}U in which the difference of the exchange Coulomb energy was found to be about 1% larger in ground state compared to its corresponding value at the top of the barrier (Le Bloas *et al.*, 2011).