The effect of atomic electrons on nuclear fission

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Abstract – We calculate the correction to the nuclear fission barrier produced by the atomic electrons. The result presented in analytical form is convenient to use in future nuclear calculations. The atomic electrons have a small stabilizing effect on nuclei, increasing the lifetime in the nuclear fission channel. This effect may be used to study the fission process.

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Introduction. – In this paper we consider the effect of atomic electrons on nuclear fission. This effect is small for all known nuclei. However, it might still be detectable. For example, the lifetime of the $^{256}$Fm ($Z = 100$) isotope, for which fission is the main decay channel (the branching ratio is 91.90% [1]) is known to four digits: $\tau = 157.6 \text{ min}$ [1]. On the other hand, our estimations show that the effect of atomic electrons on the probability of fission is about 0.2% (see below) which is on the same level of accuracy.

The effect can be observed by comparing fission probabilities of nuclei stripped from all electrons with those in neutral atoms. This may reveal important information about fission. The effect is expected to play a more significant role in the fission of superheavy nuclei leading to an increased lifetime of the nuclei. The study of the superheavy elements is now a popular area of research due to the search for the hypothetical stability island ($Z = 114$ to 126) and good progress in the synthesis of the elements on accelerators up to $Z = 118$ (see, e.g., reviews [2–5]). It is natural to expect that the physics of the superheavy nuclei has some phenomena which never manifest themselves for lighter nuclei.

In this paper we argue that for the purpose of calculating the total energy of atomic electrons the change of the nuclear shape during the fission process can be reduced to the change of the nuclear radius. We perform relativistic atomic many-body calculations of the total electron energy as a function of the nuclear radius $r_N$ and the nuclear charge $Z$. The results are fitted by an analytical formula. We also give very rough estimations of the effect of changing the electron energy on the probability of nuclear fission. More accurate estimations would probably need sophisticated nuclear calculations. The change of the total electron energy during fission found in the present work might be useful for these future nuclear calculations.

Fission and atomic electrons. – Nuclear fission is an important decay channel for heavy nuclei [6,7]. During the fission a nucleus goes through several stages of deformation before the separation of the fragments. The process is accompanied by the nuclear rotation. The rotation is fast on the timescale of the orbiting electrons. Therefore, electrons are not sensitive to the details of the change in the nuclear shape. They only feel nuclear charge density averaged over the nuclear rotation. This means that any change of the nuclear shape can be reduced to the change of the nuclear radius. This nuclear charge density for a spinless nucleus is spherical. For a non-zero nuclear spin there is an electric quadrupole moment correction which is negligible anyway. Here there is the difference with the muon case considered in ref. [8]: the muon is inside the nucleus, so the calculation in the rotating (frozen nucleus) frame is appropriate.

Therefore, the change of the electron energy during the fission process is similar to the well-known volume (or field) isotope shift of atomic transition frequencies which is determined by a change of a single nuclear parameter, mean squared nuclear charge radius. The change of the electron energy with increasing nuclear radius is positive. This means that electrons take some energy from the process making fission more difficult.

We stress that in this work we do not perform any nuclear calculations. A real shape of the fission barrier is complicated, with several minima, and an accurate calculation would require sophisticated nuclear codes. However, to explain the relevant physics and to find out if the measurements are feasible we start from presenting

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some rough estimates using a simplest parabolic barrier model (fig. 1) [6,7]. The probability of the tunneling through the barrier is given by [7]

\[ P = \frac{1}{1 + \exp \left( \frac{2\pi |U_B - E|}{\hbar \omega} \right)} , \]  

where \( U_B \) is the maximum of the potential energy (point B in fig. 1) and \( \hbar \omega \) is the potential barrier width. The width is of the order from 0.5 to 1 MeV [7]. For the spontaneous fission the tunneling amplitude is very small. Indeed, according to ref. [6] \( U_B - U_A \approx 5 \) MeV. Therefore, 

\[ 2\pi |U_A - U_B| / \hbar \omega \gg 1 \]

and

\[ P \approx \exp \left( -2\pi |U_B - E| / \hbar \omega \right) \equiv P_0 \]

for energies not too close to \( U_B \). To estimate the effect of electrons on nuclear fission we should take into account the electron energy \( E_e(\alpha) = E_e(\alpha_A) + k(\alpha - \alpha_A) + \ldots \), where \( \alpha \) is the deformation parameter (see fig. 1). The constant \( E_e(\alpha_A) \) does not change the probability of the tunneling since the constant potential does not influence the wave function (the bound-state energy \( E \) and the potential \( U \) change by the same amount \( E_e(\alpha_A) \) so the difference \( E - U_B \) does not change). The linear term \( k(\alpha - \alpha_A) \) can be incorporated into the effective parabolic potential and slightly changes the difference \( E - U_B \). Indeed, it vanishes at the point of minimum \( \alpha = \alpha_A \) where the bound state is located, and modify the potential near the maximum which determines the tunneling probability. A simple calculation gives the following result for the tunneling probability:

\[ P \equiv P_0 \exp \left( -2\pi \frac{\delta E}{\hbar \omega} \right) , \]

where \( \delta E = E_e(\alpha_B) - E_e(\alpha_A) \) is the change of the electron energy. This change is positive and therefore the factor in (3) is smaller than one. This means that the electrons make the probability of nuclear fission smaller.

To calculate \( \delta E \) we need to calculate the total electron energy of an atom for two different nuclear charge distributions corresponding to point A and point B (fig. 1). In light actinide atoms, e.g. \(^{236}\text{U}\), the deformation changes from 0.2 in the minimum to about 1 in the last maximum of the fission barrier (see, e.g. [6,8,9]). In heavier elements the difference is significantly smaller, about 0.2–0.4. As we mentioned above, after the averaging over nuclear rotation the charge distribution is spherically symmetric. For an estimate we assume that the change of the radius of the nuclear charge distribution from point A to point B is 10% (an accurate calculation will be discussed below). We calculate the nuclear potential by integrating the standard Fermi distribution for the nuclear density

\[ \rho(r) = \frac{C}{1 + \exp \left( \frac{r - r_N}{D} \right)} . \]

where \( D = d/4 \ln 3, d = 2.3 \) fm, \( r_N \approx 1.2(3Z)^{1/3} \) fm and \( C \) is a normalization factor defined by \( \int \rho \, dV = Z|e| \).

To find the electron energy of the atom we solve self-consistently a set of relativistic Hartree-Fock equations for single-electron orbitals (atomic units):

\[ \frac{d f_i}{d r} + \frac{\kappa_l}{r} f_i(r) - \left[ 2 + \alpha^2 (\epsilon_i - \hat{V}) \right] g_j(r) = 0, \]

\[ \frac{d g_j}{d r} - \frac{\kappa_j}{r} f_i(r) + (\epsilon_i - \hat{V}) f_i(r) = 0, \]

where \( \kappa = (-1)^{l+j+1/2}(j + 1/2), l \) and \( j \) are the angular and total electron momenta and \( \hat{V} \) is the sum of nuclear potential, found by integration of the nuclear density (4) and the self-consistent Hartree-Fock potential of atomic electrons. Index \( i \) numerates single-electron states.

The total electron energy in first order in the Coulomb interaction is given by

\[ E_{\text{total}} = \sum_{i=1}^{Z} \epsilon_i - \sum_{i<j} q(ijjj), \]

where \( \epsilon_i \) are Hartree-Fock energies (eq. (5)) of \( Z \) atomic electrons, \( q(ijjj) = q(ijjj) - q(ijjj) \) and \( q(abcd) \) is a Coulomb integral:

\[ q(abcd) = \int \int \psi_a(r_1)\psi_b(r_2)\psi_d(r_1)\psi_d(r_2) \frac{e^2}{|r_1 - r_2|} \psi_c(r_1) \psi_d(r_2) \, dr_1 \, dr_2. \]

The first-order Coulomb correction is important because it excludes the double counting of the energy of the Coulomb interaction between electrons. Indeed, the energy of the Coulomb interaction between electrons \( i \) and \( j \), is included in both \( \epsilon_i \) and \( \epsilon_j \).

The results for \( Z \) from 80 to 160 are presented in table 1. In this table we present the change of the total electron energy of the atom and the corresponding change in the fission probability when the nuclear radius changes by 10%. Corrections to the fission probabilities were calculated at \( \hbar \omega = 0.5 \) MeV using formula (3). At \( \hbar \omega = 1 \) MeV the change of the probability is about 2 times smaller, as is obvious from eq. (3). Equations (2) and (3) start to deviate significantly from each other at about \( Z = 130 \). In the vicinity of the stability island (\( Z \approx 120 \) to 130) electrons decrease the fission probability by few
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Table 1: Energy of 1s electron and total electron energy (MeV) of many-electron atoms as a function of the nuclear charge Z and nuclear radius \( r_N \). In the last column we present rough estimates of the relative change of the fission probability assuming a 10% change of the nuclear radius between points A and B; the actual increase with the nuclear charge is slower since the relative change of the radius in heavy elements is smaller than in light elements.

| Z  | \( r_N \) [fm] | Energy [MeV] | \( r_N \) [fm] | Energy [MeV] | \( \Delta_1s \) [MeV] | \( \Delta_{tot} \) [MeV] | \( |P - P_0|/P_0 \) [%] |
|----|----------------|-------------|----------------|-------------|-----------------|-----------------|---------------------|
| 80 | 6.14           | -0.083656   | -0.534682      | 7.09        | -0.083649       | -0.534664       | 0.00001             | 0.00002             | 0.02                |
| 90 | 7.75           | -0.110411   | -0.721344      | 8.53        | -0.110387       | -0.721283       | 0.00002             | 0.00006             | 0.08                |
| 100| 8.03           | -0.142969   | -0.948529      | 8.84        | -0.142908       | -0.948367       | 0.00006             | 0.00016             | 0.20                |
| 110| 8.29           | -0.183076   | -1.225050      | 9.12        | -0.182917       | -1.224613       | 0.00016             | 0.00044             | 0.55                |
| 120| 8.54           | -0.233429   | -1.563897      | 9.39        | -0.233024       | -1.562712       | 0.00041             | 0.00118             | 1.5                 |
| 130| 8.76           | -0.298439   | -1.987579      | 9.64        | -0.297409       | -1.984307       | 0.00103             | 0.00327             | 4.0                 |
| 140| 8.99           | -0.385348   | -2.538006      | 9.89        | -0.382769       | -2.528802       | 0.00258             | 0.00920             | 11                  |
| 150| 9.20           | -0.505625   | -3.289468      | 10.12       | -0.499261       | -3.263392       | 0.00636             | 0.02608             | 28                  |
| 160| 9.40           | -0.675140   | -4.345553      | 10.34       | -0.660488       | -4.278862       | 0.01465             | 0.06669             | 57                  |

The effect is large at extremely high Z leading to the doubling of the nuclear lifetime at \( Z = 160 \). The 1s electrons give about 30% of the total energy and more than a half of its change is due to the change of the nuclear radius. This is important because the total energy depends on the electron configuration and accurate calculations should include investigation which configuration corresponds to the ground state. Large contribution from the 1s electrons show that the effect of external electrons can be neglected.

Since the change of the electron energy is dominated by 1s electrons it is instructive to consider a simple picture with only one electron in the 1s state. The change of its energy due to the change of the nuclear radius is very small. Therefore it is natural to try the perturbation theory. The first-order correction to the Coulomb energy can be written as

\[
\Delta E(r_N) = -e \int (\phi - Z e/r) \psi^2 (r) dV, \tag{7}
\]

where \( \phi \) is the nuclear potential corresponding to the finite nuclear radius \( r_N \). The change of the energy due to the small change of the nuclear radius can be found as the difference

\[
\delta (\Delta E) = \Delta E(r_{NB}) - \Delta E(r_{NA}). \tag{8}
\]

Here \( r_{NA} \) and \( r_{NB} \) are nuclear radii at points A and B of fig. 1. The results for the relative change of the energies of 1s electrons for different Z obtained with the use of the relativistic Coulomb wave functions in eq. (7) are presented in the second column of table 2. The change of nuclear radius is 10% and the radii are the same as in table 1. The third column of table 2 presents similar results which were obtained by replacing the Coulomb wave functions with the numerical solutions of the Dirac equation corresponding to finite nuclear radius. The results are very close for small Z but deviate significantly for higher Z. This actually means that the perturbation theory does not work in spite of the fact that the correction to the energy is very small. The reason for this is very simple: the perturbation is not small but it is localized in the very small volume of space limited by the nuclear radius. Indeed, only the nuclear volume contributes to the integral (7). The finite nuclear radius dramatically changes the electron wave function inside this volume. In the end we use accurate numerical calculations rather than the perturbation theory to find the change of the electron energy due to the change of the nuclear radius.

In the fourth column of table 2 we present the results of the numerical solution of the Dirac equation with the finite nuclear size. These results are in good agreement with the data in the previous column. The energy shift is dominated by the s-wave electrons. Note that the single-electron s-wave energy shift due to finite nuclear size can be approximated by a semi-empirical formula which is accurate to few per cent from \( Z = 1 \) up to \( Z = 100 \):

\[
\Delta E_s \approx \left\{ \frac{E_{0s}}{\nu} \right\}^2 \left( \frac{2Z^2 N}{\delta_o} \right)^{2\gamma}, \tag{9}
\]
where \( \nu \) is the effective principal quantum number 
\( \nu = Z_{\text{eff}} \sqrt{a_{\text{u}} / (2E_0)} \); 
\( Z_{\text{eff}} = Z, \nu = 1 \) for the 1s state 
in the Coulomb field; 
\( Z_{\text{eff}} = 1, \nu \sim 1.7 \) for an external 
electron in a neutral atom), 
\( \gamma = \sqrt{1 - (Za)^2}, a_0 \) is the Bohr radius. 
If the change of the radius is small 
\( \delta r_N \ll r_N \) then eq. (9) leads to the following expression 
for the volume isotope shift:

\[
\delta(\Delta E_N) \approx \frac{|E_\nu|}{\nu} \frac{4}{5(\gamma + 1)} \left( \frac{2Zr_N}{a_0} \right)^{2\gamma} \frac{\Delta r_N}{r_N}. \tag{10}
\]

The energy shifts calculated with the use of eqs. (9) 
and (10) are presented in the last column of table 2. 
They are in good agreement with the accurate numerical 
solutions of the previous column.

To perform an accurate nuclear calculation of the fission 
probability change due to the electron potential it is 
convenient to have an analytical formula for the electron 
energy as a function of the nuclear radius. Therefore, we 
present the result of the fitting of the calculated total 
electron energy of a neutral atom as a function of the 
nuclear charge \( Z \) and nuclear radius \( r_N \):

\[
E_{\text{total}} = E_0 \left[ 1 - \frac{2}{5\gamma(\gamma + 1)} \left( \frac{2Zr_N}{a_0} \right)^{2\gamma} \times \left[ 0.416 - 0.002(Z - 100) \right] \right]. \tag{11}
\]

where \( E_0 \) does not depend on the nuclear radius:

\[
E_0 = 1.266Z^{\frac{1}{3}}(\gamma - 1)mc^2 \left[ 1 - 1.52 \times 10^{-3}(Z - 100) 
- 2.8 \times 10^{-5}(Z - 100)^2 \right]. \tag{12}
\]

These formulas can be used in the nuclear calculations of the 
fission process. Note that here we assume eq. (4) for 
the nuclear charge density \( \rho(r) \) averaged over the nuclear 
rotation. This formula contains the fixed parameter \( D \) 
and the variable parameter \( r_N \). Nuclear fission calculations 
operate with different variable parameters (e.g., the 
deformation parameters). Relation between \( r_N \) and these 
parameters may be easily established by a numerical 
comparison of the mean squared nuclear charge radii. 
It is assumed that nuclear physicists calculate \( r_N \) for each 
intermediate state of the nucleus during the fission process 
and then calculate the nuclear response to the electron 
potential for a given \( r_N \). To avoid misunderstanding, one 
does not need to calculate the fission lifetime to high 
accuracy to make use of the electron effect. One should 
only calculate the (relative) change of the lifetime when 
the electron potential is added.

The effect of electrons on the alpha and the proton 
emission barriers are much smaller. However, one can use 
the same eqs. (11), (12) to estimate them.

Here we assume that the experiment consists in a 
comparison of the fission probabilities for a bare nucleus 
and a neutral atom. If necessary, we can provide the result 
for an ion with an arbitrary number of electrons.

**Conclusion.** – In conclusion we state that we have 
also calculated the total electron energy of heavy and 
superheavy atoms due to a change of nuclear radius 
and fitted the results with a simple analytical formula. 
This formula can be used in nuclear calculations to include 
the effect of atomic electrons on the probabilities of nuclear 
fission. Simple estimates based on the parabolic fission 
barrier show that although the effect is small it is probably 
detectable in some nuclei. The small value of the effect has 
its advantage: it is enough to consider a linear response of 
a nucleus to the probe — the small \( r_N \)-dependent part of 
the potential produced by the atomic electrons.

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