SELF-CONSISTENT DESCRIPTION OF ALPHA DECAY PROCESS AND ATTENDANT ELECTRON SHELL EVOLUTION

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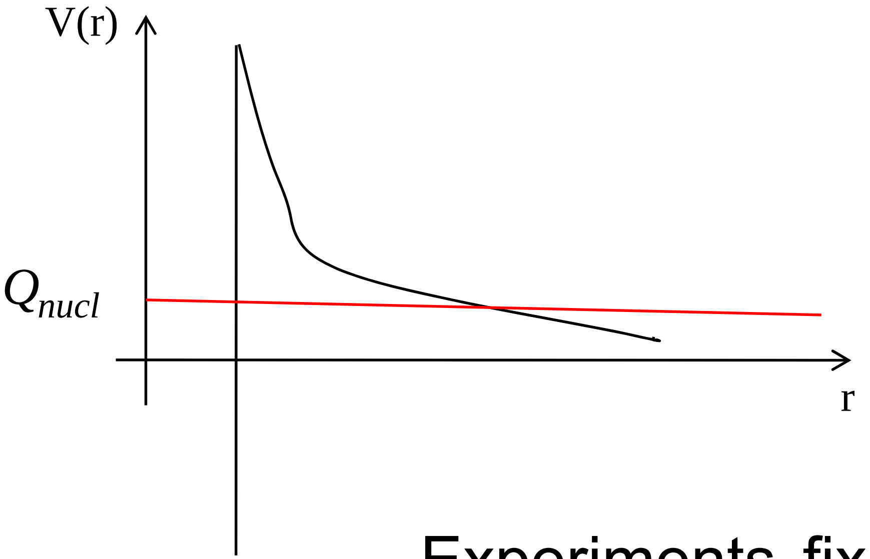
ALPHA DECAY OF A NUCLEUS



$$\Gamma_\alpha = S_\alpha (\hbar\omega/\pi) P_\alpha$$

$$P_\alpha = \exp\left[-\frac{2\sqrt{2\mu}}{\hbar} \int_{r_{\text{int}}}^{r_{ext}} \left(\sqrt{V(r) - Q_{nucl}} \right) dr \right]$$

Experiments fix the energy of α-decay of an atom. The potential of the electron shell decreases this energy compare to initial one.

The energy loss ΔE is about 40 keV for actinides. Due to that P_α changes by few tens per cent.

1. V. A. Erma, Phys. Rev. **103**, 1784 (1952).

An example of the formula:

$$\Delta E = 64.3 Z^{7/5} - 80 Z^{2/5} (keV)$$

SETTING UP OF THE PROBLEM

To consider the alpha-decay of the atom and the respective bare nucleus and to calculate the relations between the characteristics of these processes, namely the difference of the energy yields

$$\Delta E = Q_{bn} - Q_{at}$$

and the ratio of the alpha decay widths or more expressive value

$$\delta\Gamma/\Gamma = (\Gamma_{at} - \Gamma_{nucl})/(\Gamma_{at} + \Gamma_{nucl})$$

It is also interesting for the proton and the cluster decay. A supporting result

2. V. L. Mikheev et al, PEPAN Lett. 5, 623 (2008).

is the difference between the widths of ^{212}Po decay in Pb and Ni matrixes:

$$T_{1/2}(Pb) - T_{1/2}(Ni) = (-0.66 \pm 0.25)\, ns; \quad T_{1/2} = 0.3\, \mu s$$

THE PRESENT STATE OF THE ART

The discussed problem is of certain interest. A number of papers are published in the last decade:

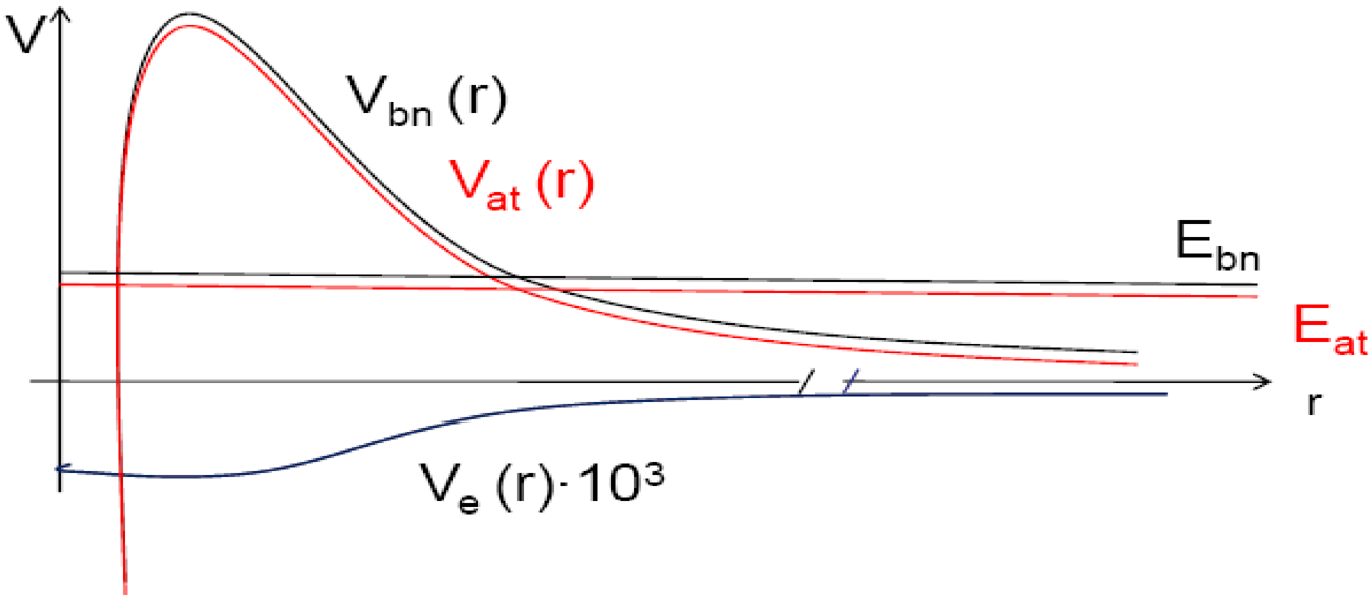
3. W. Rubinson and M. L. Perlman, Phys. Lett. B 40, 352 (1972).
4. N. T. Zinner, Nucl. Phys. A 781, 81 (2007).
5. Z. Patyk, H. Geissel, Y. A. Litvinov, A. Musumarra, and C. Nociforo, Phys. Rev. C 78, 054317 (2008).
6. S.Yu. Igashov, Yu.M. Tchuvil'sky, Phys. At. Nucl. 76, 1452, (2013).
7. F. F. Karpeshin, Phys. Rev. C 87, 054319 (2013).
8. A.Ya. Dzyublik, Phys. Rev. C 90, 054619 (2014).
9. S.Yu. Igashov, Yu.M. Tchuvil'sky, Proceedings of IASEN-2013. World Scientific .Singapore (2013) p. 191.

All these papers contain some elements of accurate formalism but no one of them aggregates all. Some significant details are skipped in all these papers.

STANDARD APPROACH. IMPACT OF THE ADDITIONAL POTENTIAL

In the WKB approximation:

$$P_{at}/P_{bn} = \exp\left[-\frac{2\sqrt{2\mu}}{\hbar}\int_{r_{\mathrm{int}}}^{r_{ext}}\left(\sqrt{V_{bn}(r)-E_{at}+V_e(r)}dr\right)-\int_{r_{\mathrm{int}}}^{r_{ext}}\left(\sqrt{V_{bn}(r)-E_{bn}}\right)dr\right]$$



$\delta\Gamma/\Gamma = P_{at}/P_{bn} - 1$ here.

QUESTIONS CALL FOR ANALYSIS

1. Is WKB approximation correct?
2. Is the reflection effect significant in the classically allowed area?
3. Does the form of the strong potential play a role?
4. Is the Thomas-Fermi model satisfactory?
5. Can one use non-relativistic approach?
6. Does finite-range distribution of nuclear charge play a role?
7. Is the process diabatic or adiabatic one in relation to the motion of electrons?
8. Does the rearrangement of the electron shell play an important role?
9. What is the probability of the electron to be knocked out?
10. Is the alpha particle bare or dressed?
11. Is the effect measurable? How to detect the effect?

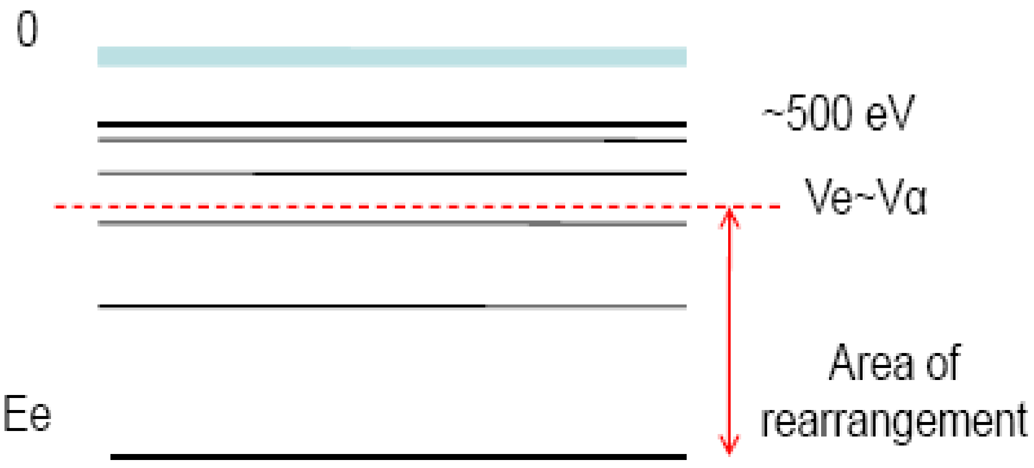
THE PROCESS PATTERN

The strongly bound electrons remain bound under the change of the nuclear charge and the weakly bound electrons are too slow to leave the shell before the α-particle. Indeed,

the equivalent electron energy

$(v_\alpha \approx v_e)$ E_e is equal

^{A}Z	E_{at}	E_e
^{144}Nd	1.9051	238
^{148}Sm	1.9858	250
^{212}Po	8.9541	1120
^{226}Ra	4.8706	690
^{232}Th	4.0828	510



The probability of a hard α-electron collision with the energy transfer E~500 eV turns out to be ~10^{-1}.

There is a partial confirmation of that by the experimental data – precisely measured energies of the emitted particles in the α-decay of 226Ra (the experimental uncertainty of the energy yield is about 250 eV) is steady but not scattered. High speed of the alpha makes it possible to consider the interaction of the alpha with two-folded negative ion of the daughter nucleus.

For the proton decay the probability of the electron knock-out or pick-up is much smaller.

So the charge of the residual system (daughter nucleus and electrons) turns out to be –2 (or –1 for the proton decay).

QUANTUM-MECHANICAL APPROACH

A pure quantum-mechanical statement of the problem of the heavy-charged-particle (proton, alpha) decay of an atom requires the following asymptotics:

$$\chi_r(r) \sim G_l(\tilde{\eta}, \tilde{k}r) + iF_l(\tilde{\eta}, \tilde{k}r), \; \textit{where} \;\; \tilde{\eta} = \alpha Z_{res} Z_2 \sqrt{\mu c^2 /(2E)}$$

Where Z_{res} is the charge of residual system (daughter nucleus and residual electrons). For the bare nucleus η is related to the charge of the daughter nucleus Z_1.

Consequently starting from this asymptotic form backward to the short distances (deep sub-barrier area, the strong forces are disappeared, the electron charge inside is negligible) one can obtain:

$$\bar{\chi}_r(r) \sim AG_l(\eta, kr) + BF_l(\eta, kr)$$

but not

$$\chi_r(r) \sim G_l(\eta, kr) + iF_l(\eta, kr)$$

At the same time at the short distances :

$$\bar{\chi}_r(r) \sim AG_l(\eta, kr) + BF_l(\eta, kr) \cong AG_l(\eta, kr).$$

because

$$F_l(\eta, kr)/G_l(\eta, kr) \cong P = \frac{2\sqrt{2\mu}}{\hbar}\int_r^{r_{ext}} \sqrt{V(\rho) - E}\, d\rho, \ \ as \ \ r \ll r_{ext};$$

and $P_{r(\mathrm{int})} \sim 10^{-17}$ for $t_{1/2} = 1\,ms.$

So the mathematical problem is to determine the multiplier A.

To do that two pairs of independent solutions of a Hamiltonian in two regions of the variation of *r* are used. They are:

$$G_l\left(\tilde{\eta},\tilde{k}r\right);\quad F_l\left(\tilde{\eta},\tilde{k}r\right)-$$

at the short distances and

$$G_l\left(\eta,kr\right);\quad F_l\left(\eta,kr\right)-$$

in the outer asymptotic region. Because of that the solution of the equation within the intermediate interval of *r* is equivalent to a linear transformation of the coefficients determining the weights of related functions in one and another regions. This transformation is described by the unimodular matrix ||M|| of the rank 2. Thus it is convenient to solve equation

$$H\chi_r\left(r\right)=E\chi_r\left(r\right).$$

where

$$H = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{Coul}(r) + V_{shell}(r) + V_{c.f.}(r).$$

with short-distance boundary

$$\chi_{reg}(r) = F_l(\eta, kr).$$

Its asymptotics at infinity takes the form:

$$\chi_{reg}(r) \sim \alpha G_l(\tilde{\eta}, \tilde{k}r) + \beta F_l(\tilde{\eta}, \tilde{k}r).$$

This solution is equivalent to the transformation:

$$\| M \| \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \Delta^{-1} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}; \quad \Delta = k / \tilde{k}$$

i. e.

$$M_{12} = \alpha / \Delta; \quad M_{22} = \beta / \Delta.$$

The inverse transformations

$$\| M^{-1} \| \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \quad and \quad \| M^{-1} \| \begin{pmatrix} 0 \\ i \end{pmatrix} = \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

allow one to obtain the multiplier A and the final result:

$$A_1 = -\alpha / \Delta; \quad A_2 = \beta / \Delta; \quad A = \sqrt{\alpha^2 + \beta^2} / \Delta.$$

$$\Gamma_{bn} / \Gamma_{at} = \frac{k}{\tilde{k}} A^2 = (\alpha^2 + \beta^2) / \Delta = \frac{\tilde{k}}{k} (\alpha^2 + \beta^2).$$

In the precise quantum-mechanical approach

$$\Gamma_{bn} / \Gamma_{at} = 0.99812423.$$

In the WKB approach

$$\Gamma_{bn} / \Gamma_{at} = 0.99812444.$$

The accurate quantum-mechanical calculations performed here demonstrate that in spite of great difference of the boundary conditions that is not taken into account by WKB approach this approximations turns out to be perfect.

DYNAMICS OF THE ALPHA PARTICLE PROPOGATION AND ENERGY FUNCTIONAL

The models using for calculations of the energy functional ***V_{shell} (r)*** in different papers vary in:

1. Methods of calculation of the electron wave functions (Thomas-Fermi, Hartree-Fock, Hartree-Fock-Dirac).
2. Scenarios of the process (diabatic – wave function of the electron shell is fixed and thus remains the same as that of the parent atom, adiabatic – it is considered to be the same as that of daughter one, two outer electrons turns out to be forgotten.

Papers [7,9] demonstrate that the results obtained by use of Hartree-Fock-Dirac model differ essentially from the ones obtained using Thomas-Fermi or Hartree-Fock ones. So the former approach is only valid.

In reality the motion of the alpha particle is adiabaic as related to fast electrons ($v_e > v_\alpha$) and diabatic as related to others. So the rearrangement of the former ones should be taken into account.

Strongly bound (and consequently fast) electrons make a dominating impact on the outgoing alpha-particle wave. The influence of two outer electrons is negligible. That is why adiabatic model looks better than diabatic.

Nevertheless, accurately speaking, a hybrid model describing fast and slow electrons in different ways is preferable.

But there is a problem of adiabatic approach. It was indicated in [5] that the energy difference

$$\Delta\Delta E = B(Z) - B(Z-2) - B(2) - V_e(0)$$

exists, where *B(Z)* is the binding energy of a respective atomic shell and $V_e(0)$ is the potential of alpha – electron shell interaction in the initial state. The origin is the rearrangement of the electron shell of the mother atom to the shell of daughter one. It must be taken into account both for the calculation of Δ*E* and, as a consequence, indirectly, Γ. The authors proposed to add this energy to the alpha-particle energy.

Unfortunately in reality the switching of the regime is not instantaneous – the electron shell evolves during the propagation of the alpha particle through it.

FORMALISM

The Hamiltonian of the system has the form:

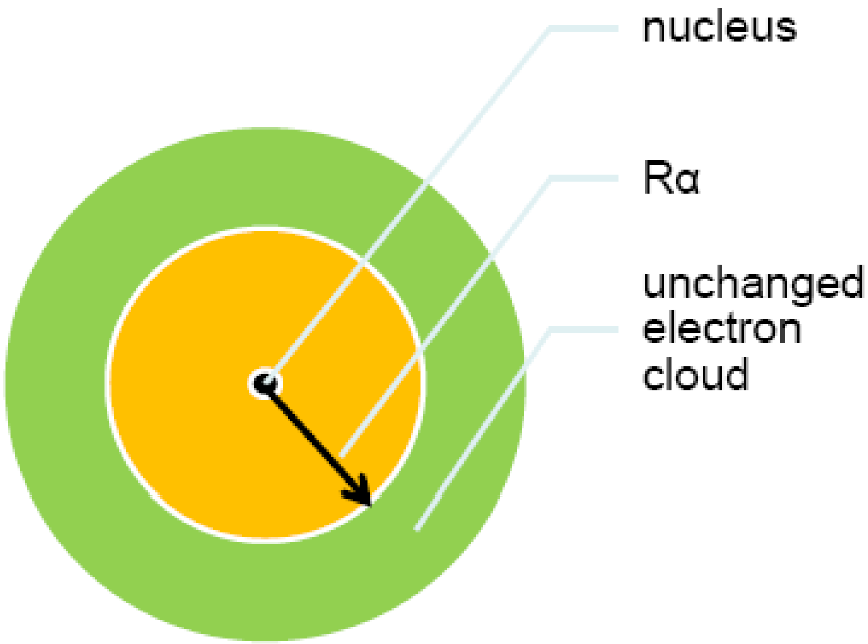
$$H = T_\alpha + V_{\alpha,(Z-2)}(r_\alpha) + T_e + V_{e,(Z-2)} + V_{\alpha,e} + V_{e,e}.$$

The interaction between the alpha and the electron (point-like volume with the charge 1) is expressed as

$$V_{\alpha,e(1)}\left(r_{\alpha,e(1)}\right) = -2e_0^2 \frac{1}{r_{\alpha,e(1)}} = -2e_0^2 \sum_L^\infty \sum_{m=-L}^{L} \frac{4\pi}{2L+1} \cdot \frac{r_<^L}{r_>^{L+1}} \cdot Y_{Lm}^*(\Omega_1) Y_{Lm}(\Omega_2).$$

In the monopole approximation

$$\Delta V\left(r_\alpha, r_{e(1)}\right) = -2e_0^2 \left(\frac{1}{\max\{r_{e(1)}, r_\alpha\}} - \frac{1}{r_{e(1)}} \right) = -2e_0^2 \begin{pmatrix} \frac{1}{r_\alpha} - \frac{1}{r_{e(1)}} & r_{e(1)} < r_\alpha \\ 0 & r_{e(1)} > r_\alpha \end{pmatrix}$$



Because of that the electrons which are located outside the sphere r_α remain to be in their initial states. The wave functions of these electrons and their desity turn out to be unchanged. The wave functions of the internal electrons are brought to the orbitals of the daughter atom. So the density is taken in the form

$$\rho(r) = \begin{pmatrix} \rho^{final}(r) & r < r_\alpha \\ \rho^{initial}(r) & r > r_\alpha \end{pmatrix}$$

$$\rho(r) = \sum_{(i)} \left|\phi_{(i)}(r)\right|^2$$

The electron wave functions are calculated by use of Hartree-Fock-Dirac approach. The Hamiltonian is written in the form:

$$\hat{H} = \sum_{i=1}^{Z} \hat{H}_i^D + \frac{1}{2}\sum_{i\neq j}^{Z} \frac{1}{r_{ij}},$$

where

$$\hat{H}^D = \hbar c(\alpha\, p) + (\beta - 1)mc^2 + V_{en}(r).$$

Its matrix element

$$\left\langle a\mu_a \,|\, \hat{H}^D \,|\, b\mu_b \right\rangle = \delta_{\mu_a\mu_b}\,\delta_{\kappa_a\kappa_b} \left\langle a \,|\, \hat{H}_r^D \,|\, b \right\rangle$$

where

$$\hat{H}_r^D = \begin{pmatrix} \hat{V}_{en}(r) & \hbar c\left(\dfrac{d}{dr} + \dfrac{\kappa}{r}\right) \\ \hbar c\left(-\dfrac{d}{dr} + \dfrac{\kappa}{r}\right) & \hat{V}_{en}(r) - 2mc^2 \end{pmatrix}$$

$$\kappa = \pm\left(J + \frac{1}{2}\right)$$

It is convenient to present the wave function of an orbital by the form of bi-spinor:

$$\phi_{n_r Jm\kappa} = \begin{pmatrix} \mathcal{G}_{n_r,\kappa}(r)\Omega_{\kappa}^{m}(\theta,\varphi) \\ i\mathcal{F}_{n_r,\kappa}(r)\Omega_{-\kappa}^{m}(\theta,\varphi) \end{pmatrix},$$

where

$$\Omega_{\kappa}^{m}(\theta,\varphi) = \sum_{m}\sum_{m_\sigma} C_{lm,1/2m_\sigma}^{J\mu} Y_{lm}(\theta,\varphi)\chi_{m_\sigma}(\sigma).$$

The expression of the electron density reads

$$\rho(r) = \sum_{i}(2J_i+1)\left(\left|\mathcal{G}_i\right|^2 + \left|\mathcal{F}_i\right|^2\right).$$

The total nucleus-electron interaction and the interaction of the alpha and the shell as a whole take the following forms:

$$\bar{V}_{e,(Z-2)}(r_\alpha) = (Z-2)e_0^2 \left(\int\limits_{r<r_\alpha} \frac{\rho^{final}(r)}{r} d^3r + \int\limits_{r>r_\alpha} \frac{\rho^{initial}(r)}{r} d^3r \right);$$

$$\bar{V}_{\alpha,e}(r_\alpha) = 2e_0^2 \left(\int\limits_{r<r_\alpha} \frac{\rho^{final}(r)}{r} d^3r + \frac{1}{r_\alpha} \int\limits_{r>r_\alpha} \rho^{initial}(r) d^3r \right).$$

The formula of the kinetic energy of the electrons reads:

$$\bar{T}_e(r_\alpha) = \sum_i (2J_i+1) \int_0^{r_\alpha} dr \left(\hbar c \cdot P_i^* \left(-\frac{d}{dr} + \frac{\kappa_i}{r} \right) Q_i + \hbar c \cdot Q_i^* \left(\frac{d}{dr} + \frac{\kappa_i}{r} \right) P_i - 2m_e c^2 \left| Q_i \right|^2 \right),$$

where

$$\mathcal{G}_i = \frac{P_i}{r}, \quad \mathcal{F}_i = \frac{Q_i}{r}.$$

Finally the alpha-particle motion in the electron shell is described by the following two-body Hamiltonian:

$$\bar{H} = T_\alpha + V_{\alpha,(Z-2)}(r_\alpha) + \bar{V}_{\alpha,e}(r_\alpha) + \bar{W}(r_\alpha),$$

where

$$\bar{W}(r_\alpha) = \bar{T}_e(r_\alpha) + \bar{V}_{e,(Z-2)}(r_\alpha) + \bar{V}_{e,e}(r_\alpha).$$

So the properties of this motion are characterized by the energy

$$Q_{at} = Q_{nucl} + \Delta E,\ \Delta E = \bar{V}_{\alpha,e}(0) + \bar{W}(0)$$

where ΔE is the energy transfer; and the penetrability

$$P_{at} / P_{bn} = \exp - \left[\frac{\dfrac{2\sqrt{2\mu_{at}}}{\hbar} \displaystyle\int_{r_{\mathrm{int}1}}^{r_{ext1}} \sqrt{V_{\alpha,(Z-2)}(r_\alpha) + \bar{V}_{\alpha,e}(r_\alpha) + \bar{W}(r_\alpha) - Q_{at}}\, dr +}{\dfrac{2\sqrt{2\mu_{bn}}}{\hbar} \displaystyle\int_{r_{\mathrm{int}2}}^{r_{ext2}} \sqrt{V_{\alpha,(Z-2)}(r_\alpha) - Q_{bn}}\, dr} \right].$$

QUALITATIVE PROPERTIES OF THE EFFECT

While the interaction potential of the alpha and the electron shell $\bar{V}_{\alpha,e}(r_\alpha)$ increases monotonically the functional $\Delta\bar{W}(r_\alpha)$ drops down and thus provides the grows of the penetrability.

The energy transfer form the shell to the alpha-particle is relatively small, $\Delta\Delta E$ =713 eV but observable because for 226Ra decay the energy yield is measured with the higher accuracy 4870.63±0.25 keV

QUANTITATIVE RESULTS. PHYSICAL EFFECTSOF THE ELECTRON SHELL

"Initial" model

1. The continuous evolution of the electron shell of the atom and permanent energy between it and the alpha particle as this particle propagates through the shell is taken into account.

2. Hartree-Fock-Dirac formalism considering the atomic nucleus as a finite-range object is explored to describe this evolving system.

3. The alpha particle is considered to be bare at the moment of fly out form the electron shell.

4. The binding energies of two redundant electrons in the daughter atom are believed to be close to zero. At the same time these electrons are slow and therefore the alpha particle leaves the interaction area earlier than them.

5. The reduced mass difference peculiar to the decay of an atom and the respective bare nucleus is neglected.

6. Twofold character of the regime of alpha-particle penetration through the electron shell which is adiabatic relative to the motion of strongly bound electrons and diabatic relative to the motion of loosely bound ones is not taken into account and purely adiabatic scenario is assumed in the approximation.

The values of E_{at} (MeV), ΔE (keV) and $\delta\Gamma/\Gamma(10^{-3})$

^{A}Z	E_{at}	ΔE_a	$\delta\Gamma_a/\Gamma_a$	$\delta\Gamma_b/\Gamma_b$	ΔE_c	$\delta\Gamma_c/\Gamma_c$
^{144}Nd	1.9051	20.853	2.675	14.521	21.337	-2.385
^{148}Sm	1.9858	21.944	2.865	14.187	22.439	-2.639
^{212}Po	8.9541	35.887	0.153	3.089	36.568	-0.252
^{226}Ra	4.8706	38.859	1.921	6.537	39.572	-2.560
^{232}Th	4.0828	40.418	3.722	7.053	41.145	-5.331

In the case that the nuclei are considered as a point-like objects the values ΔE and δΓ/Γ turn out to be equal to 20.854 keV and $2.789 \cdot 10^{-3}$ for 144Nd and 38.874 keV and $2.627 \cdot 10^{-3}$ for 226Ra decay respectively.

In the case that non-relativistic Hartree-Fock model is explored, the values ΔE and δΓ/Γ are equal to 19.553 keV and $1.608 \cdot 10^{-3}$ for 144Nd alpha decay and to 33.874 keV and $0.662 \cdot 10^{-3}$ for 226Ra respectively. Thus non-relativistic approach is in fact inadequate.

BASIC RESULTS

The values of E_{at} (MeV), ΔE (keV) and δΓ/Γ(10^{-3}) and mean excitation energy E* (eV)

^{A}Z	ΔE_{ad}	$\delta\Gamma_{ad}/\Gamma_{ad}$	ΔE_{s-ad}	$\delta\Gamma_{s-ad}/\Gamma_{s-ad}$	E^{*}
^{144}Nd	20.853	2.241	20.923	2.235	70
^{148}Sm	21.944	2.434	22.018	2.426	74
^{212}Po	35.887	-0.019	36.054	-0.023	167
^{226}Ra	38.859	1.680	38.958	1.668	99
^{232}Th	40.418	3.452	40.518	3.435	100

$$P_{at}/P_{bn}=\exp\left[-\frac{2\sqrt{2\mu_{at}}}{\hbar}\int_{r_{\mathrm{int}1}}^{r_{ext1}}\sqrt{V_{\alpha,(Z-2)}(r_\alpha)+\bar{V}_{\alpha,e}(r_\alpha)+\bar{W}(r_\alpha)-Q_{at}}\,dr+\frac{2\sqrt{2\mu_{bn}}}{\hbar}\int_{r_{\mathrm{int}2}}^{r_{ext2}}\sqrt{V_{\alpha,(Z-2)}(r_\alpha)-Q_{bn}}\,dr\right].$$

The electron shell make the reduced mass larger for the “atomic” case so this effect make the decay slower.

The process is not purely adiabatic – the velocity of the alpha particle is higher than the velocity of the outer electrons. So the energy yield calculated in the adiabatic approach is in fact the upper limit.

Because of the conservative behavior of the slow electrons the final state of the daughter atom is not an eigenstate of the atomic Hamiltonian so this atom ejects two or more electrons and turns out to be excited after that. Therefore one can expect the emission of soft X-rays and/or ultraviolet radiation.

CONCLUSIONS.
THE QUESTIONS AND THE ANSWERS

1. Is WKB approximation correct? Yes.

2. Is the reflection effect significant in the classically allowed area? The effect is negligible.

3. Does the form of the strong potential play a role? No, the result is not affected by a reasonable variation of the internal turning point.

4. Is the Thomas-Fermi model satisfactory? Direct calculations demonstrate that the answer is no.

5. Can one use non-relativistic approach? No.

6. Does finite-range distribution of nuclear charge play a role? Yes.

7. Is the process diabatic or adiabatic one in relation to the motion of electrons? The truth is somewhere in between but the accurate adiabatic approach provide a good description of the quantitative characteristics of the decay.

8. Does the rearrangement of the electron shell play an important role? Yes, the role of the rearrangement and the energy transfer accompanying it in the aggregate electron shell impact on alpha-decay widths is decisive.

9. What is the probability of the electron to be knocked out? Calculations demonstrate that the probability is rather small.

10. Is the alpha particle bare or dressed? The probability to pick-up an electron by alpha particle is small. In addition a neutral He atom can not be detected.

11. Is the effect measurable? How to detect the effect? Probably yes.

There is an example in which proton and alpha are in competition. In that case the branching ratio but not the half-life can be the object of measurements. This example is ^{160}Re isotope.

Decay	Q_{at}(MeV)	Percentage	ΔQ(keV)
$^{160}Re \rightarrow p$	1.290	91	15.19
$^{160}Re \rightarrow \alpha$	6.699	9	30.38

Another way is to measure the branching ratio of the alpha decay fine structure.

0. Is not the subject matter of the discussed investigations of solely academic interest?

Basic prospects of the developed approach may be found beyond the examples of the alpha decay of ions in laboratory conditions.

The large scale effects of such a type may appear in high electron density mediums: stars, etc.

Besides that the accumulated experience may be of advantage for the description of other nuclear processes involving the electron shell.

THANK YOU FOR ATTENTION!