ELECTRON SHELL IMPACT ON THE ALPHA-DECAY OF HEAVY NUCLEI

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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

\[ \Delta Q = Q_{bn} - Q_{at} \]

and the ratio of the alpha decay widths

\[ \frac{\Gamma_n}{\Gamma_a} \]

or a more expressive value

\[ \frac{\delta \Gamma}{\Gamma} = \frac{\Gamma_{at} - \Gamma_{nuc}}{\Gamma_{at} + \Gamma_{nuc}} \]

It is also interesting for the proton and the cluster decay.

This statement by no means reduced to the prescription to use an accurate \( Q_{bn} \) value recalculated from the experimental alpha-particle energy for the calculation of the width.
THE PRESENT STATE OF THE ART

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


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.
In the WKB approximation:

\[ \frac{P_{at}}{P_{bn}} = \exp \left[ -\frac{\sqrt{2\mu}}{\hbar} \int_{r_{int}}^{r_{ext}} \left( \sqrt{V_{bn}(r) - E_{bn}} + V_e(r) - \sqrt{V_{bn}(r) - E_{bn}} - V_e(0) \right) \, dr \right] \]

\[ \delta \Gamma / \Gamma = \frac{P_{at}}{P_{bn}} - 1 \text{ here.} \]
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. Is the process diabatic or adiabatic one in relation to the motion of electrons?
7. Does the rearrangement of the electron shell play an important role?
8. What is the probability of the electron to be knocked out?
9. Is the alpha particle bare or dressed?
10. 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,

$$v_\alpha (v_p) \approx v_e \quad \text{at} \quad E_e = 500 \text{ eV}$$

The probability of a hard α-electron collision with the energy transfer $E \sim 500 \text{ eV}$ turns out to be $\sim 10^{-1}$. 
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).
A pure quantum-mechanical statement of the problem of the heavy-charged-particle (proton, alpha) decay of an atom requires the following asymptotics:

\[ \chi_r(r) \sim G_i(\tilde{\eta},\tilde{k}r) + iF_i(\tilde{\eta},\tilde{k}r), \quad \text{where} \quad \tilde{\eta} = \alpha Z_{res} Z_2 \sqrt{\mu c^2 / (2E)} \]

Where \( Z_{res} \) is the charge of residual system (daughter nucleus and residual electrons). For the bare nucleus \( \eta \) 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:

\[ \overline{\chi}_r(r) \sim AG_i(\eta,kr) + BF_i(\eta,kr) \]

but not

\[ \chi_r(r) \sim G_i(\eta,kr) + iF_i(\eta,kr) \]
At the same time at the short distances:

\[ \tilde{\chi}_r(r) \sim AG_l(\eta, kr) + BF_l(\eta, kr) \cong AG_l(\eta, kr). \]

because

\[ F_l(\eta, kr) / G_l(\eta, kr) \cong P = \frac{1}{\hbar} \int_r^{r_{\text{ext}}} \sqrt{E - V(\rho)} d\rho, \text{ as } r \ll r_{\text{ext}}; \]

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

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:

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

at the short distances and

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

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

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

with short-distance boundary

\[ \chi_{\text{reg}}(r) = F_i(\eta, kr). \]

Its asymptotics at infinity takes the form:

\[ \chi_{\text{reg}}(r) \sim \alpha G_i(\tilde{\eta}, \tilde{kr}) + \beta F_i(\tilde{\eta}, \tilde{kr}). \]

This solution is equivalent to the transformation:

\[ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \Delta^{-1} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}; \quad \Delta = k/\tilde{k} \]

i. e.

\[ M_{12} = \alpha / \Delta; \quad M_{22} = \beta / \Delta. \]
The inverse transformations

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

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

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

$$\Gamma_{bn} / \Gamma_{at} = \frac{k}{k} A^2 = (\alpha^2 + \beta^2) / \Delta.$$
DYNAMICS OF THE ALPHA PARTICLE PROPAGATION AND ENERGY FUNCTIONAL $V_{\text{shell}} (r)$

The models using for calculations of the energy functional $V_{\text{shell}} (r)$ 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 [4,6] 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 adiabatic as compared to fast electrons ($E_e > 500$ keV) and diabatic as compared 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. Naturally, a hybrid model describing fast and slow electrons in different ways is preferable. Moreover as it indicated in [2] “instantaneous switching” to adiabatic regime result in incorrect energy balance. Indeed, in the initial state alpha is located inside the nucleus and interacts with mother electron shell while immediately after the ejection it interacts with the daughter one.
As a result the difference

\[ \Delta\Delta Q = B(Z) - B(Z - 2) - B(2) - V_e(0), \]

where \( B(Z) \) is the binding energy of a respective atomic shell, appears. It must be taken into account both for the calculation of \( \Delta Q \) and, as a consequence, indirectly, \( \Gamma \).

Unfortunately:

a) this correction to the \( \Delta Q \) value was interpreted in [2] as a physical but not recalculational effect and

b) in reality the switching of the regime is not instantaneous – the electron shell evolves during the propagation of the alpha particle through it.
The interaction of the alpha particle with the electrons is considered in the monopole approximation

\[ V_{\alpha e}(r) = 2e^2 \sum_{i} \left( \frac{1}{\max\{r_{ei}, r\}} - \frac{1}{r} \right) \]

Because of that the electrons which are located outside the sphere \( R_\alpha \) remain to be in their initial states. The wave functions of the slow electrons are considered to be fixed everywhere. The wave functions of the fast electrons are brought to the orbitals of the daughter atom.
Thus the energy functional $V_{\text{shell}}(r)$ takes the form:

$$V_{\text{shell}}(r) = \left\langle \hat{A}\{\Psi_{\text{fast}}(r)\Psi_{\text{slow}}\} \mid H_{el} \mid \hat{A}\{\Psi_{\text{fast}}(r)\Psi_{\text{slow}}\} \rightangle$$

where

$$H_{el} = \sum_i T_i + V_{Z-2}(r_{ei}) + V_{ae}(r, r_{ei}) + \sum_{i,j} V_{ee}(r_i, r_j)$$

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.
<table>
<thead>
<tr>
<th>Isotope</th>
<th>$Q_{at}$(MeV)</th>
<th>$\Delta Q$(keV)</th>
<th>$\delta \Gamma / \Gamma$(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{144}$Nd</td>
<td>1.9051</td>
<td>21.37</td>
<td>-0.25</td>
</tr>
<tr>
<td>$^{148}$Sm</td>
<td>1.9858</td>
<td>22.47</td>
<td>-0.27</td>
</tr>
<tr>
<td>$^{212}$Po</td>
<td>8.9541</td>
<td>36.62</td>
<td>-0.024</td>
</tr>
<tr>
<td>$^{226}$Ra</td>
<td>4.8706</td>
<td>39.62</td>
<td>-0.27</td>
</tr>
<tr>
<td>$^{232}$Th</td>
<td>4.0828</td>
<td>41.20</td>
<td>-0.54</td>
</tr>
<tr>
<td>$^{294}$118</td>
<td>11.75</td>
<td>72.47</td>
<td>-0.40</td>
</tr>
</tbody>
</table>
HOW TO DETECT THE EFFECT?

It is more or less clear that the search for the discussed effect could be performed by use of the storage rings of heavy ions. However the measurement of the half-life times are hard and inexact. What to do?

The idea is to explore 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.

<table>
<thead>
<tr>
<th>Decay</th>
<th>$Q_{\text{at}}$(MeV)</th>
<th>Percentage</th>
<th>$\Delta Q$(keV)</th>
<th>$\delta \Gamma/\Gamma$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{160}$Re→p</td>
<td>1.290</td>
<td>91</td>
<td>15.19</td>
<td>−0.41</td>
</tr>
<tr>
<td>$^{160}$Re→α</td>
<td>6.699</td>
<td>9</td>
<td>30.38</td>
<td>−0.21</td>
</tr>
</tbody>
</table>
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 rather modest.

3. Does the form of the strong potential play a role? No.


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

6. Is the process diabatic or adiabatic one in relation to the motion of electrons? The truth is somewhere in between.
7. Does the rearrangement of the electron shell play an important role? The effect of the rearrangement on the alpha decay energies, widths and residual excitation atomic energies should be taken into account.

8. What is the probability of the electron to be knocked out? The probability is rather small.

9. 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.

10. How to detect the effect? The promising way is to measure the branching ratio of the alpha and the proton decay in $^{160}$Re isotope.
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!