Alpha Decay

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1 Introduction

The half-lives of heavy elements that emit alpha particles can vary by more than 20 orders of magnitude although the energy of the emitted alpha particles only changes slightly, this strong dependence on energy suggests that the process is exponential in nature.
In this assignment, we investigate this behavior by modeling alpha decay using a numerical approach for quantum tunneling through a Coulomb barrier in one-dimension. The goal is to calculate the transmission coefficient and the corresponding half-life of ^{212}Po and ^{238}U.

2 Theory

2.1 Quantum Tunneling

In alpha decay, an alpha particle is trapped inside the nuclear potential well. According to classical mechanics, if the particle does not have sufficient energy to overcome the potential energy barrier with a height greater than the total energy of the particle, it should not be able to escape the nucleus.
However, quantum mechanics allows a probability that the particles penetrate through the barrier without sufficient energy and appear on the other side of the box.
Mathematically, when the particle reaches such barrier it can not overcome, its wave function changes from sinusoidal to exponentially diminishing in form:

$$\Psi(x) = Ae^{ik_I x} + Be^{-ik_I x} \quad \longrightarrow \quad \Psi(x) = De^{k_{II} x} + Ce^{-k_{II} x} \tag{1}$$

where A, B, C and D are constants, and k is the wave-number defined as follows:

$$k_I = \frac{\sqrt{2m(E-V)}}{\hbar}$$
$$k_{II} = \frac{\sqrt{2m(V-E)}}{\hbar}$$

2.2 Polonium-212

^{212}Po is an extremely short-lived radionuclide, it undergoes alpha decay by emitting an alpha particle and transforming into lead-208:

$$^{212}\text{Po} \quad \rightarrow \quad ^{208}\text{Pb} + \alpha \tag{2}$$

This process releases energy, Q, shared between the kinetic energies of the daughter nucleus and the alpha particle. The Q-value is given by the mass difference between the parent and the decay products:

$$Q = (M_P - M_D - M_\alpha) \cdot c^2 \approx 8.954 \text{ MeV} \tag{3}$$

Considering the decay in the center-of-mass frame, the kinetic energy can be expressed as:

$$E = \frac{1}{2} v_{rel}^2 M_\mu \tag{4}$$

where v_{rel} is the relative velocity and M_μ is the reduced mass defined as:

$$v_{rel} = v_\alpha \left(1 + \frac{M_\alpha}{M_D}\right)$$

$$M_\mu = \frac{M_\alpha M_D}{M_\alpha + M_D}$$

With the particle energy determined, it can now be compared to the potential energy of the barrier to determine the appropriate form of the wave function in each region, as described in Section 2.1.
Enforcing the continuity of the wave function and its derivative across the boundary gives the amplitudes of incoming, reflected, and transmitted waves:

$$1 = R + T = \frac{|B|^2}{|A|^2} + \frac{|F|^2}{|A|^2}\frac{k_{III}}{k_I} \tag{5}$$

Where R and T is the Reflection and Transmission coefficients respectively, those values are then used to calculate the decay constant as follows [1]:

$$\tau = \frac{2R}{Tv} \tag{6}$$

Using this along with the Radioactive decay law, the half-life was computed as follow :

$$t_{1/2} = \tau \ln 2 \tag{7}$$

2.3 Uranium-238

On the other extreme, ^{238}U is a extremely long-lived radionuclide, it undergoes alpha decay into ^{234}Th with the emission of an alpha particle:

$$^{238}\mathrm{U} \rightarrow {}^{234}\mathrm{Th} + \alpha \tag{8}$$

The energy released in this decay is calculated similarly:

$$Q \approx 4.2749\ \ \mathrm{MeV} \tag{9}$$

Although this energy is only slightly lower than that of Po-212, we will see that it effects the half-life dramatically due to its exponential dependence.

[1] Modeling the α particle bouncing backwards and forwards inside the nucleus of radius R with some speed v presumably related to its energy.

3 Numerical solution

3.1 Important Parameters

To approach this problem numerically, we approximate the Coulomb potential barrier by dividing it into a finite number of segments of equal length, each having a constant potential, allowing the wave function to be expressed as a linear combination of exponential terms within that region.

A number of parameters must be calculated for this model, the most important one being the length of the potential barrier, which range from the nuclear radius, R_N, to some maximum radius, R_{max}.
Since the nuclear influence is assumed to stop when the emitted alpha and the reduced nucleus are just touching each other, the distance R_N can easily be calculated using the nuclear radius relation (calculations made using parameters for Po-212):

$$R_N = R_0 A^{1/3} \approx 1.2 \ \cdot \ (4^{1/3} + 208^{1/3}) \approx 9.01 \text{ fm} \tag{10}$$

The particle will escape the barrier when its energy exceeds the energy of the Coulomb potential barrier, $Q = V_C$. Using that, we can force the particle to escape at the last segment and hence the distance R_{max} can be calculated as follows:

$$\alpha Z_1 Z_2 \frac{\hbar c}{R_{max}} \approx 8.954 \text{ MeV} \quad \rightarrow \quad R_{max} \approx 26.9 \text{ fm} \tag{11}$$

Having the necessary parameters, we can now construct the full solution by enforcing the continuity of both the wave function and its derivative at each boundary between segments. This results in a system of linear equations which can be written in matrix form:

$$\boldsymbol{AX} = \boldsymbol{B} \tag{12}$$

where $\boldsymbol{X}$ contains the unknown coefficients we need to find for each region, which were solved using numpy.linalg.solve() function.

3.2 Testing the code

To verify the implementation several tests were done, in particular, we:

- Checked that $R + T \approx 1$ for all configurations.
- Verified convergence of the solution by increasing the number of barrier segments N.
- Tested that the exponential behavior is observed only inside the potential barrier.

3.3 Limitations of the model

While our numerical approach gave good insights into the tunneling process in alpha decay, it involves a couple of simplifications and approximations, those fall into two main categories:

3.3.1 Physical limitations

Simplified potential model In our model, we approximated the nuclear potential with a square well with fixed depth, and the Coulomb barrier using discrete constant steps. While in reality, both the strong nuclear potential and the electrostatic potential vary smoothly with distance, hence, this sharp boundaries we model between regions are not physically accurate and introduces small discrepancies in the wavefunction behavior.

Neglect of angular momentum This model assumes the emitted alpha particle has zero angular momentum ($\ell = 0$), ignoring the centrifugal barrier term in the potential:

$$V_\ell(r) = \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} \tag{13}$$

Therefore, in real life problems where the decays involves non-zero angular momentum, this additional barrier would reduce the tunneling probability and increase the half-life.

3.3.2 Numerical limitations

Segment resolution and Computational costs The accuracy of the stepwise barrier approximation depends on the number of segments N. The smaller the N, the less accurate the results are, so increasing N improves resolution but also leads to a larger linear system and hence increased computational cost. Hence, one has to find a balance point where the results are considered good enough without sacrificing a lot of unnecessary computational resources.

Exponential instability The wavefunction under the barrier decays exponentially over many orders of magnitude, and this rapid decay is captured in the form of complex exponentials in the matrix system. Hence, in certain matrix rows both exponentially growing and decaying terms appear simultaneously, which can cause numerical instability.

4 Results

4.1 Po-212

Solving equation (10) and extracting the coefficients corresponding to the first and last region, the half-life time was found using equation (7):

$$t_{1/2} \approx 363 \text{ ns} \tag{14}$$

Compared to the experimental value of about 300 ns, this represents a small overestimation, but still a good agreement given the simplicity of the model, this discrepancy can be attributed to the limitations discussed in Section 3.3.
The last step to verify our numerical approach is a visual one:

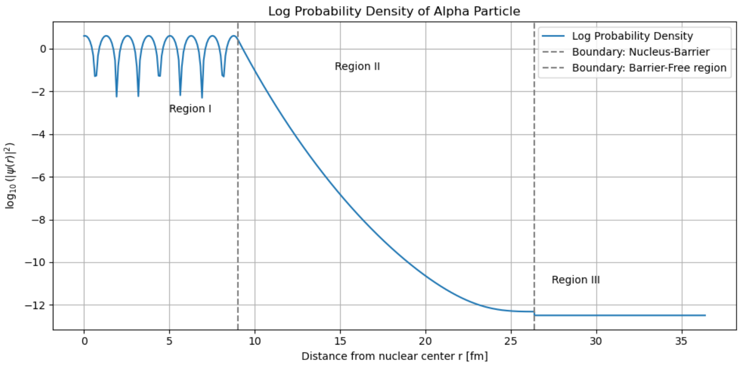

Figure 1: The Log-probability density of the alpha particle in the decay of ^{212}Po.

The plot above shows the logarithm of the probability density as a function of distance from the nuclear center. In region I, inside the nucleus, the strong nuclear force dominates and the wavefunction exhibits oscillatory behavior due to the particle being in a classically allowed region. The relatively high and constant probability density reflects the particle being confined within the potential well.
In region II, the particle tunnels inside the classically forbidden region under the Coulomb barrier, the wave function decays exponentially, which is evident as a linear drop on the logarithmic scale.
Beyond the barrier, region III, the wavefunction flattens out at a very low value, indicating that a small fraction of the wavefunction has tunneled through.

4.2 U-238

The numerical simulation was repeated for ^{238}U, with this relatively small change in the alpha particles energy, the tunneling probability becomes extremely small leading to a calculated half-life on the order of:

$$t_{1/2} \approx 13 \cdot 10^9 \text{ years} \tag{15}$$

This is fairly consistent in magnitude with the known experimental value which ($\sim$ 4.5 billion years), the discrepancy is acceptable given the model's assumptions and simplifications [2]

[2]Note that only **79% of ^{238}U nuclei** decay to the ground state of ^{234}Th. This affects the interpretation of the half-life calculated here.

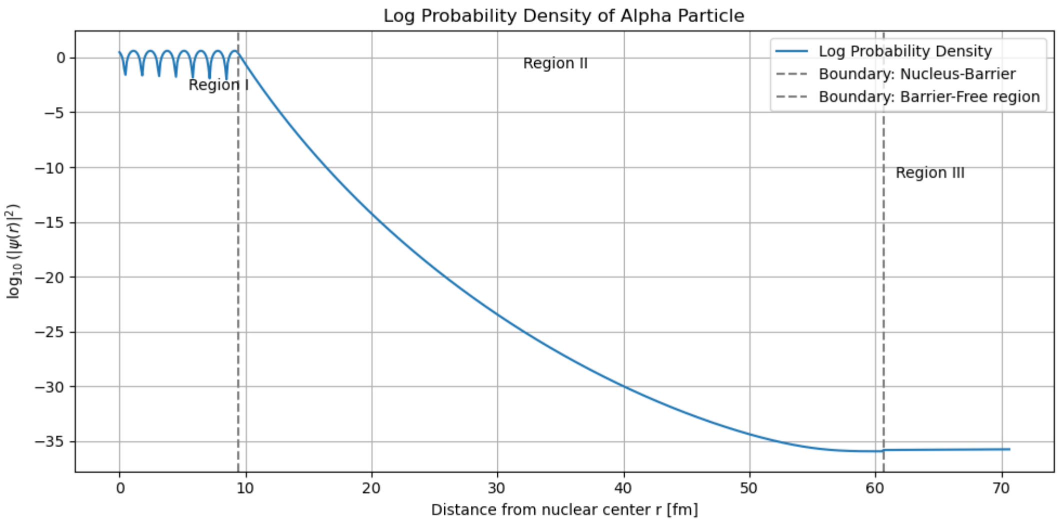

Figure 2: The Log-the probability density for the alpha particle in the decay of ^{238}U.

We can directly observe in Figure 2 that the wavefunction plots for ^{238}U and ^{212}Po share the same qualitative features, oscillatory behavior inside the nucleus, exponential decay under the barrier and a small transmitted wave beyond the barrier.
However, the key difference lies in the steepness of the exponential decay, for ^{238}U, the wavefunction drops by over 35 orders of magnitude, and consequently a much lower tunneling probability and a significantly longer half-life.

5 Discussion and conclusions

The simulation successfully models the quantum tunneling process involved in alpha decay of ^{212}Po and ^{238}U. By approximating the Coulomb barrier with discrete potential steps and solving the Schrödinger equation at each segment numerically, we obtained the wavefunctions across the three relevant regions. Figure 1 and 2 clearly shows how the relatively small decrease in alpha energy causes the half-life to increase by many orders of magnitude —from ns in the case of ^{212}Po to billions of years for ^{238}U–.