

Can tunnelling solve the α -decay puzzle?

This is the information that should have been given during the class - on the black board. Read and do the evaluations yourself in order to understand.

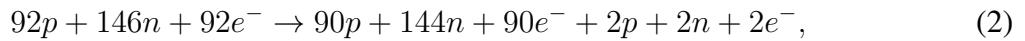
- The puzzle: Why is there such a life-time variation when nuclei decay by α -emission.

The kinematics of the decay

An example of α -decay is:



Looking at all the particles (neutrons, protons, electrons) involved we have:



The number of particles are the same - but there is a difference in *binding energy*. The available energy

$$M_P c^2 \rightarrow M_D c^2 + M_\alpha c^2 + E_{kin}. \quad (3)$$

(P=parent nucleus D=Daughter nucleus). Looking up the masses in some Table we will see that:

$$M_P c^2 > M_D c^2 + M_\alpha c^2, \quad (4)$$

which is necessary for the decay to happen.

Experiments are conducted in the lab-frame, but we start to look at the decay in the center-of-mass frame. There the parent nucleus is at rest before the decay, and thus the momentum of the reaction products add to zero as well

$$M_D v_D + M_\alpha v_\alpha = 0 \rightarrow v_D = -\frac{M_\alpha}{M_D} v_\alpha. \quad (5)$$

and the kinetic energy after the decay will be:

$$E_{kin} = \frac{1}{2} M_D v_D^2 + \frac{1}{2} M_\alpha v_\alpha^2 \quad (6)$$

This is the energy released in the decay.

Decay means that the α -particle leaves the daughter nucleus. An important quantity is thus the *relative velocity*:

$$v_{rel} = v_\alpha - v_D = v_\alpha \left(1 + \frac{M_\alpha}{M_D} \right) \quad (7)$$

and we may rewrite the kinetic energy in terms of relative velocity:

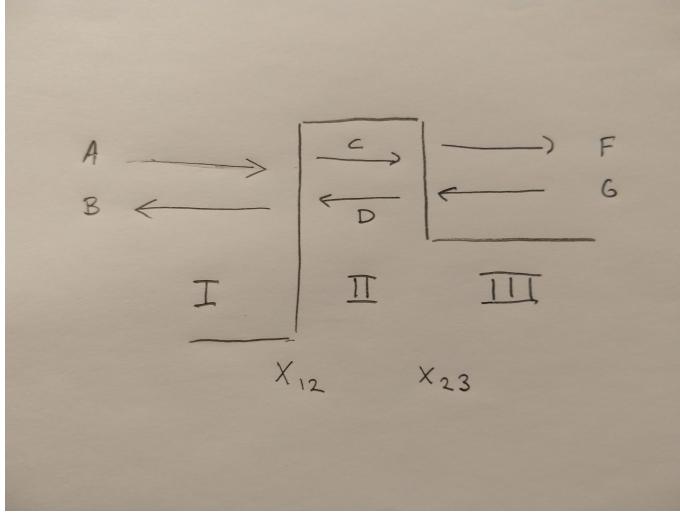


Figure 1: The simple case with one potential barrier

$$\begin{aligned}
 \frac{1}{2}M_\alpha v_\alpha^2 + \frac{1}{2}M_D v_D^2 &= \frac{1}{2}M_\alpha v_\alpha^2 \left(1 + \frac{M_\alpha}{M_D}\right) \\
 \frac{1}{2}M_\alpha v_\alpha^2 \left(1 + \frac{M_\alpha}{M_D}\right) &= \frac{1}{2}M_\alpha v_{rel}^2 \left(1 + \frac{M_\alpha}{M_D}\right)^{-1} \\
 \frac{1}{2}M_\alpha v_{rel}^2 \left(1 + \frac{M_\alpha}{M_D}\right)^{-1} &= \frac{1}{2}v_{rel}^2 \left(\frac{M_\alpha M_D}{M_D + M_\alpha}\right) \\
 E_{kin} &= \frac{1}{2}v_{rel}^2 M_\mu
 \end{aligned} \tag{8}$$

where the reduced mass is defined as :

$$M_\mu = \left(\frac{M_\alpha M_D}{M_D + M_\alpha}\right) \tag{9}$$

What do we know about tunnelling?

Gamov's idea was that quantum mechanical tunneling could explain why small differences in energy release can lead to large differences in life time.

We start to repeat what we know about tunnelling and begin with the textbook case with one barrier in one dimension.

Tunnelling: Just one barrier, and in one dimension

This is a short account - your QM book probably has more detailed discussions.

The starting point is the Schrödinger equation. If $V = \text{konst}$ it says:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) = (E - V)\Psi(x) \tag{10}$$

if $(E - V) > 0$ the solution is:

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}, k = \sqrt{2m(E - V)}/\hbar \tag{11}$$

while if $(E - V) < 0$ we have:

$$\Psi(x) = Ce^{kx} + De^{-kx}, k = \sqrt{2m(V - E)/\hbar} \quad (12)$$

Now we have three regions. In the first and third regions the particle energy is exceeding the potential energy $(E - V_I) > 0$, $(E - V_{III}) > 0$, but in the middle region $(E - V_{II}) < 0$. The solutions in the three regions will then be

$$\Psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x} \quad (13)$$

$$\Psi_{II}(x) = Ce^{k_{II}x} + De^{-k_{II}x} \quad (14)$$

$$\Psi_{III}(x) = Fe^{ik_{III}x} + Ge^{-ik_{III}x} \quad (15)$$

$$(16)$$

where A, B, C, D are constants. From the time-dependent Schrödinger we can find the expression for probability flux (this is discussed in most QM books if you have to repeat it). The expression for the flux through a point x_0 is

$$\frac{i\hbar}{2m} \left(\Psi^*(x) \frac{\partial\Psi(x)}{\partial x} - \Psi(x) \frac{\partial\Psi^*(x)}{\partial x} \right)_{x=x_0} \quad (17)$$

If $\Psi(x) = ae^{\pm ikx}$ then the probability flux is

$$\mp |a|^2 \frac{k\hbar}{m} \quad (18)$$

where the signs tells us if the flux is from left to right (minus sign since the flux is decreasing to the left of the boarder) or from right to left (plus sign since the flux is increasing to the left of the boarder).

Considering now particles scattered on the barrier from the left (and not from the right), we watch what is coming into and going out from the potential barrier (region II). The inward flux through x_{12} , the boarder between region I and II, is then

$$|A|^2 \frac{\hbar k_I}{m} \quad (19)$$

and the outward through x_{12}

$$- |B|^2 \frac{\hbar k_I}{m}. \quad (20)$$

Through x_{23} we have an outward flux of

$$|F|^2 \frac{\hbar k_{III}}{m}. \quad (21)$$

Nothing comes in from the right, giving us that $G = 0$.

If nothing is absorbed in the barrier everything that goes in must go out:

$$|A|^2 \frac{\hbar k_I}{m} - |B|^2 \frac{\hbar k_I}{m} = |F|^2 \frac{\hbar k_{III}}{m} \quad (22)$$

divide with the first term (and move the B term to the right-hand side) and you find

$$1 = \left| \frac{B}{A} \right|^2 + \left| \frac{F}{A} \right|^2 \frac{k_{III}}{k_I} = R + T, \quad (23)$$

where R is the reflected fraction and T the transmitted fraction of the incoming particles. So we have four unknowns $B/A, C/A, D/A$, and F/A , or putting $A=1, B, C, D, F$.

There is also something more which we know about the solution: Since we need to be able to take the second derivative of the wave function everywhere (the Schrödinger equation) both the wave function itself and the first derivative should be continuous everywhere, i.e. also at the boundaries between the three regions.

$$Ae^{ik_I x_{12}} + Be^{-ik_I x_{12}} - Ce^{k_{II} x_{12}} - De^{-k_{II} x_{12}} = 0 \quad (24)$$

$$Ce^{k_{II} x_{23}} + De^{-k_{II} x_{23}} - Fe^{ik_{III} x_{23}} = 0 \quad (25)$$

$$ik_I A e^{ik_I x_{12}} - ik_I B e^{-ik_I x_{12}} - k_{II} C e^{k_{II} x_{12}} + k_{II} D e^{-k_{II} x_{12}} = 0 \quad (26)$$

$$k_{II} C e^{k_{II} x_{23}} - k_{II} D e^{-k_{II} x_{23}} - ik_{III} F e^{ik_{III} x_{23}} = 0 \quad (27)$$

That is four equations for the four unknowns. We can put this in matrix form

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ e^{ik_I x_{12}} & e^{-ik_I x_{12}} & -e^{k_{II} x_{12}} & -e^{-k_{II} x_{12}} & 0 \\ ik_I e^{ik_I x_{12}} & -ik_I e^{-ik_I x_{12}} & -k_{II} e^{k_{II} x_{12}} & +k_{II} e^{-k_{II} x_{12}} & 0 \\ 0 & 0 & e^{k_{II} x_{23}} & e^{-k_{II} x_{23}} & -e^{ik_{III} x_{23}} \\ 0 & 0 & k_{II} e^{k_{II} x_{23}} & -k_{II} e^{-k_{II} x_{23}} & -ik_{III} e^{ik_{III} x_{23}} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ F \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (28)$$

That is we have an equation of the form

$$\mathbf{AX} = \mathbf{B} \quad (29)$$

The next step is to generalize to many barriers. With N there are $2N$ unknowns in the barriers, one unknown in the well (the reflected wave), and one unknown outside (the final transmitted wave). Total $2N + 2$ unknowns. $N + 1$ boarders, each with two conditions gives $2N + 2$ equations.

- The task is to construct the matrix, solve the system of linear equations and find the transmission coefficient T

How to get the life time

- The transmission coefficient gives the probability for an incident particle to get out. How do we translate that to a lifetime?

Think like this: inside the well the particle has an energy E_{kin} corresponding to a velocity v it travels back and fourth and hits the wall every time. That is with a frequency $v/2R$. Thus the probability that it gets out per unit time is $T \times v/2R$ (with T being the transmission coefficient).

$$\frac{1}{\tau} = T \frac{v}{2R} \quad (30)$$

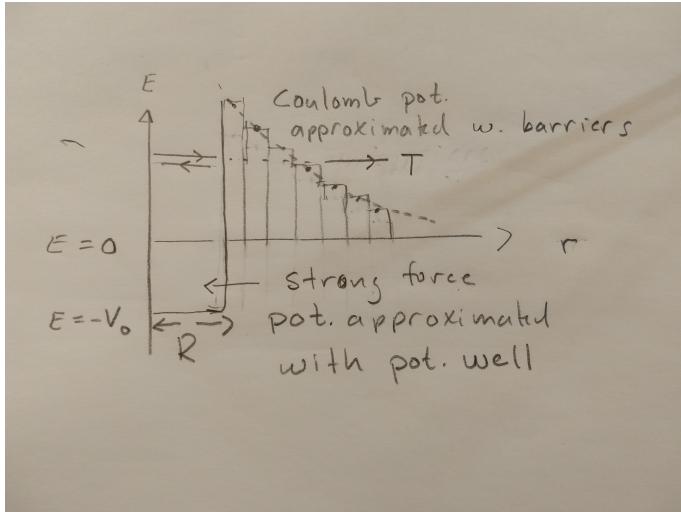


Figure 2: The model.

Half-life

$$N(t) = N_0 e^{-t/\tau} \quad (31)$$

$$N(t_{1/2}) = \frac{N_0}{2} \quad (32)$$

$$e^{-t_{1/2}/\tau} = \frac{1}{2} \quad (33)$$

$$-\frac{t_{1/2}}{\tau} = \ln\left(\frac{1}{2}\right) \quad (34)$$

$$t_{1/2} = \tau \ln(2) \quad (35)$$

Some advices for the units

In nuclear physics masses are often given in MeV/c^2 , energies in MeV, and distances in $10^{-15}\text{m} = 1 \text{ fm}$. For a free particle

$$E = \frac{\hbar k^2}{2m} \quad (36)$$

and thus

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2mc^2E}}{\hbar c} \quad (37)$$

If we use MeV for mc^2 and E and for $\hbar c = 197.3269631\dots \text{ MeV} \times \text{fm}$ That is energy times length. we get k in fm^{-1} . The Coulomb repulsion can also be cast in a convenient form:

$$\frac{e^2 Z_1 Z_2}{4\pi\epsilon_0} \frac{1}{r} = Z_1 Z_2 \frac{e^2}{4\pi\epsilon_0 \hbar c} \frac{\hbar c}{r} = \alpha Z_1 Z_2 \frac{\hbar c}{r} \quad (38)$$

$\alpha = e^2/(4\pi\epsilon_0 \hbar c) = 1/137.035399\dots$ is the fine structure constant. Use $\hbar c$ as above and r in fm, and the result is in MeV.

System of Linear equations

The numerical problem in this assignment will be in the form of a matrix equation . This is a common problem which has been studied a lot

$$\mathbf{AX} = \mathbf{B} \quad (39)$$

A standard method is Gauss-elimination with back substitution (which you probably have encountered in your numerical method course. Routines for such general methods are available. You do not need to program them yourselves, but it is good to know something about how they work.

To start with one transforms the matrix to upper tridiagonal form i.e.:

$$\mathbf{A} \rightarrow \begin{pmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & 0 & x \end{pmatrix} \quad (40)$$

With a small matrix one can follow the method step by step:

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \quad (41)$$

that is:

$$a_{11}x_1 + a_{12}x_2 = b_1 \quad (42)$$

$$a_{21}x_1 + a_{22}x_2 = b_2. \quad (43)$$

$$a_{11}x_1 + a_{12}x_2 = b_1 \quad (44)$$

$$a_{21}x_1 + a_{22}x_2 - (a_{21}/a_{11})(a_{11}x_1 + a_{12}x_2) = b_2 - (a_{21}/a_{11})b_1 \quad (45)$$

$$a_{11}x_1 + a_{12}x_2 = b_1 \quad (46)$$

$$\left(a_{22} - \frac{a_{21}a_{12}}{a_{11}} \right) x_2 = b_2 - (a_{21}/a_{11})b_1 \quad (47)$$

Multiply the first equation with (a_{21}/a_{11}) and subtract from the first equation

$$\begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22} - \frac{a_{21}a_{12}}{a_{11}} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 - (a_{21}/a_{11})b_1 \end{pmatrix} \quad (48)$$

$$\begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22}^{(2)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2^{(2)} \end{pmatrix} \quad (49)$$

For more dimensions the upper tridiagonal form is obtained after a number of similar actions:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} \\ 0 & 0 & 0 & a_{44}^{(4)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2^{(2)} \\ b_3^{(3)} \\ b_4^{(4)} \end{pmatrix} \quad (50)$$

with

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)} \quad (51)$$

$$b_i^{(k+1)} = b_i^{(k)} - m_{ik} b_k^{(k)} \quad (52)$$

$$m_{ik} = a_{ik}^{(k)} / a_{kk}^{(k)} \quad (53)$$

$$(54)$$

In the 2×2 matrix we get the x_i by back substitution

$$x_2 = \frac{b_2^{(2)}}{a_{22}^{(2)}} \quad (55)$$

$$x_1 = \frac{b_1}{a_{11}} - \frac{a_{12} b_2^{(2)}}{a_{11} a_{22}} \quad (56)$$

or more general

$$x_i = \frac{\left(b_i^{(i)} - \sum_{k=i+1}^n a_{ik}^{(i)} x_k \right)}{a_i^{ii}}, i = n, n-1, n-2, \dots, 1 \quad (57)$$

Obvious problems if $a_{ii} = 0$. Interchange the rows to avoid this - pivoting. This is also important for accuracy. The information about the pivoting has then to be saved! The good routines do this. We need that $\mathbf{A} \neq 0$ (non-zero determinant). If it is zero we lack one equation (perhaps because two equations are rather equal..)

Gauss elimination with back substitution need $N^3/3$ operations. How could we do better?

LU-decomposition

If you want to solve for many right-hand sides, but have the same matrix you can save a lot of time by starting with an *LU*-decompositions

If you can write your matrix \mathbf{A} as

$$\mathbf{A} = \mathbf{L}\mathbf{U} \quad (58)$$

with

$$\mathbf{U} \sim \begin{pmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & 0 & x \end{pmatrix} \quad (59)$$

is upper tridiagonal and \mathbf{L} is lower tridiagonal with unit vectors with one on the diagonal.

$$\mathbf{L} \sim \begin{pmatrix} 1 & 0 & 0 & 0 \\ x & 1 & 0 & 0 \\ x & x & 1 & 0 \\ x & x & x & 1 \end{pmatrix} \quad (60)$$

then

$$\mathbf{AX} = \mathbf{B} \quad (61)$$

$$\mathbf{L}(\mathbf{UX}) = \mathbf{B} \quad (62)$$

$$\mathbf{LY} = \mathbf{B}, \mathbf{UX} = \mathbf{Y} \quad (63)$$

$$(64)$$

Easy back substitution to get first \mathbf{Y} , and then \mathbf{X}

$$y_1 = b_1 \quad (65)$$

$$y_2 = b_2 - y_1 L_{21} \dots \quad (66)$$

This last step is just a N^2 procedure! So you get many right-hand sides for the price of one!

Can we improve the accuracy further?

We want $\mathbf{AX} = \mathbf{B}$. After solution check:

$$\mathbf{AX}_{\text{sol}} - \mathbf{B} = 0? \quad (67)$$

Probably not:

$$\mathbf{X}_{\text{sol}} = \mathbf{X}_{\text{true}} + \Delta \mathbf{X} \quad (68)$$

$$\mathbf{AX}_{\text{sol}} = \mathbf{A}(\mathbf{X}_{\text{true}} + \Delta \mathbf{X}) = \mathbf{B} + \Delta \mathbf{B} \quad (69)$$

$$\mathbf{AX}_{\text{true}} + \mathbf{A}\Delta \mathbf{X} = \mathbf{B} + \Delta \mathbf{B} \quad (70)$$

$$\mathbf{A}\Delta \mathbf{X} = \Delta \mathbf{B} \quad (71)$$

$$\mathbf{A}\Delta \mathbf{X} = \mathbf{AX}_{\text{sol}} - \mathbf{B} \quad (72)$$

See Numerical Recipes 2.5 (page 55). Solve for $\Delta \mathbf{X}$ to get an estimate of the error which can be used to improve the result! If you have done an LU decomposition this is really cheap!!

Program packages

Implementations of these methods are (freely) available through the *Linear Algebra PACKage (LAPACK)*, which is written in Fortran 90. It provides routines for systems of linear equations, eigenvalue problems, and singular value problems etc. LAPACK is integrated in e.g. Mathematica or Matlab and can be accessed with Python. See links on the course web page (Athena). There is a C interface and a Windows version.

C-users might think that it is easier to use (Eigen) - instead of LaPack. Eigen is a C++ template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms - it is tested against LaPack.

You will use such standard solvers for several Assignments during the course. High-level languages as Matlab can select by itself which version of a solver to use. Low-level languages such as C or Fortran leave this to you. It is more complicated, but allows for more optimization and eventually faster performance for large problems. There exist different routines for real single, real double, complex single, complex double matrices, as well as for real symmetric, hermitian and banded matrices.

For the α -decay Assignment you need a system of linear equation solver. For example

dgesv (Double precision, General matrix, Equation System)

zgesv (Complex Double precision, General matrix, Equation System)

dgbsv (Double precision, General matrix, Banded Equation System)

dsysv (Double precision, General matrix, Equation System)

Here you will have a complex matrix and it is better to use double precision.

The routines usually do a *LU* decomposition, but if you want to make full use of the approach and just do the *LU* decomposition once there are also routines which separate the *LU* decomposition from the solutions of the system of linear equation, for example for a Complex Double precision General matrix.

`zgetrf` - perform LU-decomposition

`zgetrs` - solves the system with the LU factorized form.

The LAPACK routines use the BLAS - Basic Linear Algebra Sub-program routines which makes all basic matrix operation go faster. If you are running on a multi-core machine you can use Math Kernel Library (MKL) which parallelize the matrix operations - and you do not need to change the code at all.