Physics GR6037

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10/27/2025

The decay of an unstable state using Schrödinger quantum mechanics and the WKB approximation

As was discussed in class the α-decay of a highly charged nucleus can be described by the potential shown in Fig. 1.

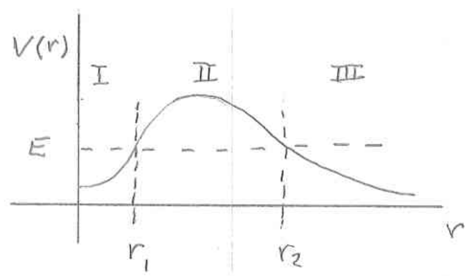

Figure 1: Potential seen by an alpha particle as it moves in the vicinity of a highly charged nucleus to which it would be bound were it not for the large Coulomb repulsion.

We will use the WKB approximation to show how exponential decay occurs in this context. We will work with an angular momentum eigenstate assumed to have $\ell = 0$ and solve the radial Schrödinger equation:

$$\left\{-\frac{\hbar^2}{2m}\partial_r^2 + V(r)\right\} u_E(r) = E u_E(r) \tag{1}$$

working with a radial wave function $u_E(r)$ obtained by multiplying the usual Schrödinger wave function by r. Thus, $u_E(r)$ must vanish at the origin and except for very special energies the wave function in region I will be a sum of sines and cosines which will connect to a WKB solution in region II which grows exponentially as r increases. Since the barrier separating regions I and III is not infinitely high, all Schrödinger eigenfunctions will be non-zero in region III, the energy spectrum will be continuous with the solutions in region III being a sum of incoming and scattered outgoing plane waves. We will normalize the solutions $u_E(r)$ using a delta function of the energy:

$$\int_0^\infty u_{E'}(r) u_E(r) dr = \delta(E' - E). \tag{2}$$

To obtain $u_E(r)$, we will start with two WKB solutions that do not obey the boundary condition at the origin but are a sine or cosine in region III. The first is intended to be small in regoin I and to connect to an increasing exponential in region II and then to the usual sine function in region III.

$$u_S(r) = \begin{cases} \frac{1}{\sqrt{v(r)}}\frac{T^{\frac{1}{2}}}{2}\cos\left(-\frac{1}{\hbar}\int_0^r p(r')dr' + \eta\right) = \frac{1}{\sqrt{v(r)}}\frac{T^{\frac{1}{2}}}{2}\cos\left(\frac{1}{\hbar}\int_r^{r_1} p(r')dr' + \frac{\pi}{4}\right) & 0 \le r \le r_1 \\ \frac{1}{\sqrt{|v(r)|}}\frac{T^{\frac{1}{2}}}{2}\exp\left(\frac{1}{\hbar}\int_{r_1}^r |p(r')|dr'\right) = \frac{1}{2}\frac{1}{\sqrt{|v(r)|}}\exp\left(-\frac{1}{\hbar}\int_r^{r_2} |p(r')|dr'\right) & r_1 \le r \le r_2 \\ \frac{1}{\sqrt{v(r)}}\sin\left(\frac{1}{\hbar}\int_{r_2}^r p(r')dr' + \frac{\pi}{4}\right) & r_2 \le r \end{cases} \tag{3}$$

where η and T are given by:

$$\eta = \frac{1}{\hbar}\int_0^{r_1} p(r)dr + \frac{\pi}{4} \tag{4}$$
$$T = \exp\left(-\frac{2}{\hbar}\int_{r_1}^{r_2} |p(r)|dr\right). \tag{5}$$

To use the connection formulae properly when deriving Eq. (3), we begin in region I and then connect to region II and then to region III. The factors of $T^{\frac{1}{2}}$ have been inserted to make $u_S(r)$ have a simple normalization in region III.

A simlar use of the connection formulae begins with the solution in region III that connects to a solution increasing exponentially in region II as r decreases and leads to our second solution $u_L(r)$ which is large in region I:

$$u_L(r) = \begin{cases} \frac{1}{\sqrt{v(r)}}\frac{2}{T^{\frac{1}{2}}}\sin\left(-\frac{1}{\hbar}\int_0^r p(r')dr' + \eta\right) = \frac{1}{\sqrt{v(r)}}\frac{2}{T^{\frac{1}{2}}}\sin\left(\frac{1}{\hbar}\int_r^{r_1} p(r')dr' + \frac{\pi}{4}\right) & 0 \le r \le r_1 \\ \frac{1}{\sqrt{|v(r)|}}\frac{1}{T^{\frac{1}{2}}}\exp\left(-\frac{1}{\hbar}\int_{r_1}^r |p(r')|dr'\right) = \frac{1}{\sqrt{|v(r)|}}\exp\left(\frac{1}{\hbar}\int_r^{r_2} r|p(r')|dr'\right) & r_1 \le r \le r_2 \\ \frac{1}{\sqrt{v(r)}}\cos\left(\frac{1}{\hbar}\int_{r_2}^r p(r')dr' + \frac{\pi}{4}\right) & r_2 \le r. \end{cases} \tag{6}$$

We next combine the two approximate solutions described above to obtain the single solution $u_E(r)$ with energy E which obeys the boundary condition at the origin:

$$u_E(r) = N_E\left\{\frac{T^{\frac{1}{2}}}{2}\cos(\eta)u_L(r) - \frac{2}{T^{\frac{1}{2}}}\sin(\eta)u_S(r)\right\} \tag{7}$$

where the factor N_E is chosen so that these solutions with continuous eigenvalues are normalized to an energy delta function:

$$\int_0^\infty u_{E'}(r)u_E(r)dr = \delta(E' - E). \tag{8}$$

It is straight forward to see from the small r behavior seen in Eqs. (3) and (6) that $u_E(r) = 0$.

In order to determine the normalization factor N_E, we introduce a further parametrization of $u_E(r)$ given in Eq. (7). Define

$$W_E = \left[\left(\frac{T^{\frac{1}{2}}}{2}\cos(\eta)\right)^2 + \left(\frac{2}{T^{\frac{1}{2}}}\sin(\eta)\right)^2\right]^{\frac{1}{2}} \tag{9}$$
$$\tan(\phi_E) = \frac{\frac{T^{\frac{1}{2}}}{2}\cos(\eta)}{\frac{2}{T^{\frac{1}{2}}}\sin(\eta)}. \tag{10}$$
$$\tag{11}$$

With this notation we can easily express the large r behavior of $u_E(r)$:

$$u_E(r) = N_E W_E\left\{\sin(\phi_E)u_L(r) - \cos(\phi_E)u_S(r)\right\} \tag{12}$$
$$\underset{r_2<r}{=} \frac{1}{\sqrt{v(r)}}N_E W_E \sin\left(\frac{1}{\hbar}\int_{r_2}^r p(r')dr' + \frac{\pi}{4} - \phi_E\right). \tag{13}$$

Relying on the orthonality of the energy eigenstates of the hermitian radial Schrödinger operator, we can determine the normalization coefficient N_E by requiring that the large r behavior of $u_E(r)$ give the singular behavior required by that delta function condition. Thus, we consider

$$\begin{aligned}
\int_0^\infty u_{E'}(r)u_E(r)dr &\approx N_E^2 W_E^2 \int_0^\infty \frac{dr}{\sqrt{v'v}} \left(\frac{e^{i(\frac{p'r}{\hbar}+\theta)} - e^{-i(\frac{p'r}{\hbar}+\theta)}}{2i}\right) \\
&\qquad\qquad \times \left(\frac{e^{i(\frac{pr}{\hbar}+\theta)} - e^{-i(\frac{pr}{\hbar}+\theta)}}{2i}\right) && (14)\\
&\approx N_E^2 W_E^2 \int_{-\infty}^\infty \frac{dr}{v} \frac{e^{\frac{i(p'-p)r}{\hbar}}}{4} && (15)\\
&\approx N_E^2 W_E^2 \frac{2\pi}{4} \delta\left(\frac{p'-p}{\hbar}\right)\frac{dp}{dE} && (16)\\
&\approx N_E^2 W_E^2 \frac{2\pi\hbar}{4} \delta\left(E'-e\right) && (17)
\end{aligned}$$

where in Eq. (15) we have combined only the two terms where the r-dependent phases can cancel for $p' = p$. Equation (17) requires:

$$N_E = \frac{2}{\sqrt{2\pi\hbar} W_E}. \tag{18}$$

Examining Eq. (7) we can recognize that for most energies $\sin(\eta_E) \neq 0$ and the eigenfunction $u_E(r)$ has the expected behavior with the two terms on the right-hand side of that equation having the same size for $r < r_1$ and for larger r the exponentially growing term dominating. This requires that $N_E \sim 1/W_E$ is very small, as can be seen to be the case from Eq. (9) where $W_E \sim 1/T^{\frac{1}{2}}$. However for a special energy E_0 at which $\sin(\eta_{E_0}) = 0$, the "small" function $u_S(r)$ will be absent, $W_E \sim T^{\frac{1}{2}}$ will be small and the eigenstate $u_{E_0}(r)$ will be very large for $r < r_1$.

We now hypothesize that a radial wave function u_0 constructed from this special eigenstate $u_{E_0}(r)$ is the wave function for our decaying state:

$$u_0(r) = \begin{cases} \frac{N_0}{\sqrt{v_{E_0}(r)}} \sin\left(\eta_{E_0} - \frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right) & r < r_1 \\ 0 & r_1 < r \end{cases} \tag{19}$$

This state will be normalized if we choose the normalization factor N_0 so that

$$\begin{aligned}
1 &= \int_0^\infty u_0^2(r)dr && (20)\\
&= N_0^2 \int_0^{r_1} \frac{1}{v_{E_0}} \sin^2\left(\eta_{E_0} - \frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right)dr && (21)\\
&= N_0^2 \int_0^{r_1} \frac{1}{v_{E_0}} \frac{1}{2} dr && (22)\\
&= N_0^2 \frac{\tau_c}{4} dr, && (23)
\end{aligned}$$

where the crossing time τ_c given by

$$\tau_c = 2\int_0^{r_1} \frac{1}{v_{E_0}} dr \tag{24}$$

is the time required for the α particle to travel from one side of the nucleus to which it is almost bound to the other. Thus, $N_0 = 2/\sqrt{\tau_c}$

We can now use our energy eigenfunctions to determine the time dependence of the Schröder equation solution $u_0(r,t)$ which at $t = 0$ equals $u_0(r)$:

$$u_0(r,t) = \int_0^\infty dE\, C_E u_E(r) e^{-iEt/\hbar} \tag{25}$$

where

$$C_E \;=\; \int_0^\infty dr\, u_E(r) u_0(r), \tag{26}$$

which follows directly from our normalization of the energy eigenstates $u_E(r)$ using an energy delta function. We can combine Eqs (7) and (19) to evaluate Eq. (26) in the approximation that T is very small:

$$\begin{aligned}
&= \int_0^{r_1} dr \left[\frac{2}{\sqrt{2\pi\hbar} W_E}\left\{\frac{T^{\frac{1}{2}}}{2}\cos(\eta_E) u_L(r) - \frac{2}{T^{\frac{1}{2}}}\sin(\eta_E) u_S(r)\right\}\right] && (27)\\
&\qquad\qquad \times \left[\frac{2}{\sqrt{\tau_c}}\sqrt{v_{E_0}}\sin\left(\eta_{E_0} - \frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right)\right] \\
&\approx \int_0^{r_1} dr \left[\frac{2}{\sqrt{2\pi\hbar}} \frac{1}{\left[\left(\frac{T^{\frac{1}{2}}}{2}\cos(\eta_E)\right)^2 + \left(\frac{2}{T^{\frac{1}{2}}}\sin(\eta_E)\right)^2\right]^{\frac{1}{2}}}\left\{\frac{T^{\frac{1}{2}}}{2}\cos(\eta_{E_0}) u_L(r)\right\}\right] && (28)\\
&\qquad\qquad \times \left[\frac{2}{\sqrt{\tau_c}}\sqrt{v_{E_0}}\sin\left(\eta_{E_0} - \frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right)\right] \\
&\approx \int_0^{r_1} dr\, \frac{2}{\sqrt{2\pi\hbar}} \frac{1}{\left[\left(\frac{T^{\frac{1}{2}}}{2}\cos(\eta_E)\right)^2 + \left(\frac{2}{T^{\frac{1}{2}}}\sin(\eta_E)\right)^2\right]^{\frac{1}{2}}} && (29)\\
&\qquad\qquad \times \left\{\frac{T^{\frac{1}{2}}}{2}\cos(\eta_{E_0}) \frac{1}{\sqrt{v_{E_0}(r)}}\frac{2}{T^{\frac{1}{2}}}\sin\left(\eta_{E_0} - \frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right)\right\} \\
&\qquad\qquad\qquad \left[\frac{2}{\sqrt{\tau_c}}\sqrt{v_{E_0}}\sin\left(\eta_{E_0} - \frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right)\right] \\
&\approx \frac{2}{\sqrt{2\pi\hbar}} \frac{\cos(E_0)}{\left[\left(\frac{T^{\frac{1}{2}}}{2}\cos(\eta_E)\right)^2 + \left(\frac{2}{T^{\frac{1}{2}}}\sin(\eta_E)\right)^2\right]^{\frac{1}{2}}} \frac{2}{\sqrt{\tau_c}}\frac{\tau_c}{4} && (30)
\end{aligned}$$

where we have assumed that the factor $1/W_E$ is negligibly small unless $E \approx E_0$ so that everywhere except in this sharply peaked $1/W_E$ factor, we can replace the variable E by E_0.

We can also make a similar approximation for W_E if we use:

$$\sin\eta_E = \sin(\eta_{E_0}) + \cos(E_0)\left.\frac{d\eta_E}{dE}\right|_{E=E_0}(E - E_0) = \cos(E_0)\frac{\tau_c}{2\hbar}(E - E_0) \tag{31}$$

since

$$\frac{d\eta_E}{dE} = \frac{1}{\hbar}\frac{d}{dE}\int_0^{r_1} dr\, p_E(r)dr = \frac{1}{\hbar}\int_0^{r_1} dr\,\frac{1}{v(r)}dr = \frac{\tau_c}{2\hbar}. \tag{32}$$

Combining this equation with Eq. (30) we can write:

$$C_E \approx \frac{1}{\sqrt{2\pi\hbar}}\frac{\cos(E_0)\sqrt{\tau_c}}{\left[\frac{T}{4}+\left(\frac{2}{T^{\frac{1}{2}}}\frac{\tau_c}{2\hbar}(E-E_0)\right)^2\right]^{\frac{1}{2}}} \tag{33}$$

$$\approx \frac{1}{\sqrt{2\pi\hbar}}\frac{\cos(E_0)\frac{T^{\frac{1}{2}}\hbar}{\sqrt{\tau_c}}}{\left[\left(\frac{T\hbar}{2\tau_c}\right)^2+(E-E_0)^2\right]^{\frac{1}{2}}} \tag{34}$$

$$\approx \frac{1}{\sqrt{2\pi}}\frac{\cos(E_0)\Gamma^{\frac{1}{2}}}{\left[\left(\frac{\Gamma}{2}\right)^2+(E-E_0)^2\right]^{\frac{1}{2}}} \tag{35}$$

if we let $\Gamma = T\hbar/\tau_c$.

With this relatively simple approximate form for C_E we can work out the time dependence of our initial state u_0. We might first check that the norm of this state when evaluated using its energy wave function C_E is still unity:

$$1 \stackrel{?}{=} \int_0^\infty dE\, C_E^2 \tag{36}$$

$$\stackrel{?}{\approx} \int_{-\infty}^{\infty} dE \frac{1}{2\pi}\frac{\Gamma}{(E-E_0)^2+\left(\frac{\Gamma}{2}\right)^2} \tag{37}$$

$$\stackrel{?}{\approx} \int_{-\infty}^{\infty} dE \frac{1}{2\pi}\frac{\Gamma}{\left[(E-E_0)+i\frac{\Gamma}{2}\right]\left[(E-E_0)-i\frac{\Gamma}{2}\right]} \tag{38}$$

$$\stackrel{?}{\approx} \frac{1}{2\pi}\frac{2\pi i\Gamma}{\left[2i\frac{\Gamma}{2}\right]} \tag{39}$$

$$= 1, \tag{40}$$

if to evaluate Eq. (38) we use Cauchy's theorem to close the contour in the upper or lower half plane. In Fig. 2 we show the original path of the energy integral now extended to an approximate path between $-\infty$ and $+\infty$ and the contour C_2. The union of C_1 and C_2 is a closed contour to which Cauchy's theorem can be applied. We argue that the dominant contribution to the integral comes from the region around E_0 so extending the integral to begin at $E = -\infty$ instead of $E = 0$ does not introduce a significant error. The contribution from countour C_2 which is being added to C_1 will truly vanish in the limit that its radius increased to infinity because of the increasing denominator $\sim 1/E^2$.

Finally we can calculate the probability amplitude $A(t)$ that after a time t has elapsed the state $u_0(r,t)$ is found to be in the original state $u_0(r)$. Using Eqs. (25) and (26) we

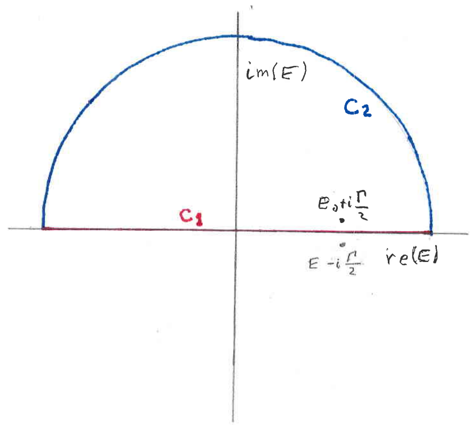

Figure 2: The complex energy plane showing the two poles at $E = E_0 \pm \frac{\Gamma}{2}$, the contour C_1 which approximates the original integration path and a second semicircular contour C_2 that can be added to C_1 in order to apply Cauchy's theorem.

find:

$$\begin{aligned} A_0(t) &= \int_0^\infty u_0(r) u_0(r,t) dr & (41)\\ &= \int_0^\infty C_E^2 \, e^{-i\frac{Et}{\hbar}} & (42)\\ &\approx \int_{-\infty}^\infty \frac{1}{2\pi} \frac{\Gamma \, e^{-i\frac{Et}{\hbar}}}{\left[(E-E_0)+i\frac{\Gamma}{2}\right]\left[(E-E_0)-i\frac{\Gamma}{2}\right]} & (43)\\ &\approx e^{-iE_0t} e^{-\frac{\Gamma t}{2\hbar}}. & (44) \end{aligned}$$

Now when closing the energy contour to obtain Eq. (44) from (43) we are forced to close the contour in the lower half plane to avoid the exponential growth of the factor $e^{-i\frac{Et}{\hbar}}$ when E has a positive imaginary part.

The magnitude squared of the amplitude $A_0(t)$ gives the probability that the particle remains in the original state u_0 at the time t

$$P_0(t) = |A_0(t)|^2 = e^{-\frac{\Gamma t}{\hbar}}. \tag{45}$$

which shows exponential decay at a rate $\Gamma/\hbar$ or with a lifetime $\tau_{\mathrm{lt}} = \hbar/\Gamma$.

We should also observe that C_E^2 gives the probability density for energy of the emitted α particle:

$$C_E^2 = \frac{1}{\sqrt{2\pi}} \frac{\Gamma}{\left(\frac{\Gamma}{2}\right)^2 + (E-E_0)^2} \tag{46}$$

Thus, the α particle is not emitted with the definite energy E_0 but instead with a distribution of energies sharply peaked around E_0. The energy distribution given in Eq. (46) can be called a Briet-Wigner distribution or Lorentzian line shape. The product of this width in energy Γ with the lifetime τ_{lt} saturates the time-energy uncertainty relation $\tau_{\mathrm{lt}}\Gamma = \hbar$.