CHAPTER 8

THE WKB APPROXIMATION

The **WKB** (Wentzel, Kramers, Brillouin)[1] method is a technique for obtaining approximate solutions to the time-independent Schrödinger equation in one dimension (the same basic idea can be applied to many other differential equations, and to the radial part of the Schrödinger equation in three dimensions). It is particularly useful in calculating bound state energies and tunneling rates through potential barriers.

The essential idea is as follows: Imagine a particle of energy E moving through a region where the potential $V(x)$ is *constant*. If $E > V$, the wave function is of the form

$$\psi(x) = Ae^{\pm ikx}, \quad \text{with } k \equiv \sqrt{2m(E - V)}/\hbar.$$

The plus sign indicates that the particle is traveling to the right, and the minus sign means it is going to the left (the general solution, of course, is a linear combination of the two). The wave function is oscillatory, with fixed wavelength ($\lambda = 2\pi/k$) and unchanging amplitude (A). Now suppose that $V(x)$ is *not* constant, but varies rather slowly in comparison to λ, so that over a region containing many full wavelengths the potential is *essentially* constant. Then it is reasonable to suppose that ψ remains *practically* sinusoidal, except that the wavelength and the amplitude change slowly with x. This is the inspiration behind the WKB approximation. In effect, it identifies two different levels of x-dependence: rapid oscillations, *modulated* by gradual variation in amplitude and wavelength.

[1] In Holland it's KWB, in France it's BWK, and in England it's JWKB (for Jeffreys).

By the same token, if $E < V$ (and V is constant), then ψ is exponential:

$$\psi(x) = Ae^{\pm\kappa x}, \quad \text{with } \kappa \equiv \sqrt{2m(V-E)}/\hbar.$$

And if $V(x)$ is *not* constant, but varies slowly in comparison with $1/\kappa$, the solution remains *practically* exponential, except that A and κ are now slowly-varying functions of x.

Now, there is one place where this whole program is bound to fail, and that is in the immediate vicinity of a classical **turning point**, where $E \approx V$. For here λ (or $1/\kappa$) goes to infinity, and $V(x)$ can hardly be said to vary "slowly" in comparison. As we shall see, a proper handling of the turning points is the most difficult aspect of the WKB approximation, though the final results are simple to state and easy to implement.

8.1 THE "CLASSICAL" REGION

The Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi,$$

can be rewritten in the following way:

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi, \qquad [8.1]$$

where

$$p(x) \equiv \sqrt{2m[E - V(x)]} \qquad [8.2]$$

is the classical formula for the momentum of a particle with total energy E and potential energy $V(x)$. For the moment, I'll assume that $E > V(x)$, so that $p(x)$ is *real*; we call this the "classical" region, for obvious reasons—classically the particle is *confined* to this range of x (see Figure 8.1). In general, ψ is some complex function; we can express it in terms of its *amplitude*, $A(x)$, and its *phase*, $\phi(x)$—both of which are *real*:

$$\psi(x) = A(x)e^{i\phi(x)}. \qquad [8.3]$$

Using a prime to denote the derivative with respect to x, we find:

$$\frac{d\psi}{dx} = (A' + iA\phi')e^{i\phi},$$

and

$$\frac{d^2\psi}{dx^2} = [A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2]e^{i\phi}. \qquad [8.4]$$

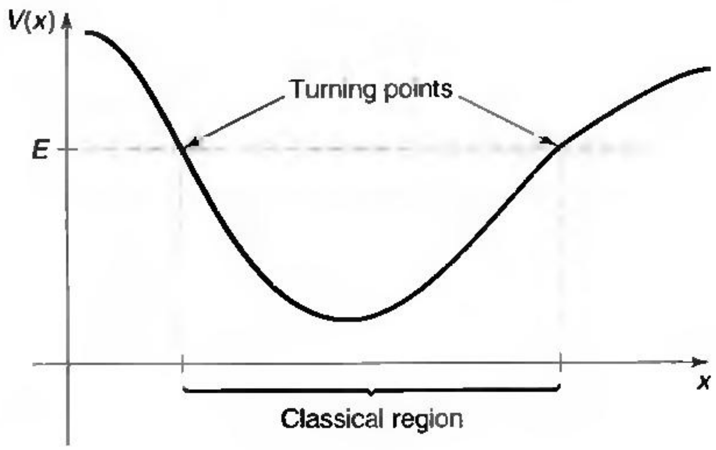

FIGURE 8.1: Classically, the particle is confined to the region where $E \geq V(x)$.

Putting this into Equation 8.1:

$$A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A. \quad [8.5]$$

This is equivalent to two *real* equations, one for the real part and one for the imaginary part:

$$A'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A, \quad \text{or} \quad A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right], \quad [8.6]$$

and

$$2A'\phi' + A\phi'' = 0, \quad \text{or} \quad \left(A^2\phi'\right)' = 0. \quad [8.7]$$

Equations 8.6 and 8.7 are entirely equivalent to the original Schrödinger equation. The second one is easily solved:

$$A^2\phi' = C^2, \quad \text{or} \quad A = \frac{C}{\sqrt{\phi'}}, \quad [8.8]$$

where C is a (real) constant. The first one (Equation 8.6) cannot be solved in general—so here comes the approximation: *We assume that the amplitude A varies slowly*, so that the A'' term is negligible. (More precisely, we assume that A''/A is much less than both $(\phi')^2$ and $p^2/\hbar^2$.) In that case we can drop the left side of Equation 8.6, and we are left with

$$(\phi')^2 = \frac{p^2}{\hbar^2}, \quad \text{or} \quad \frac{d\phi}{dx} = \pm\frac{p}{\hbar},$$

and therefore

$$\phi(x) = \pm\frac{1}{\hbar}\int p(x)\,dx. \qquad [8.9]$$

(I'll write this as an *indefinite* integral, for now—any constants can be absorbed into C, which may thereby become complex.) It follows that

$$\boxed{\psi(x) \cong \frac{C}{\sqrt{p(x)}}e^{\pm\frac{i}{\hbar}\int p(x)\,dx},} \qquad [8.10]$$

and the general (approximate) solution will be a linear combination of two such terms, one with each sign.

Notice that

$$|\psi(x)|^2 \cong \frac{|C|^2}{p(x)}, \qquad [8.11]$$

which says that the probability of finding the particle at point x is inversely proportional to its (classical) momentum (and hence its velocity) at that point. This is exactly what you would expect—the particle doesn't spend long in the places where it is moving rapidly, so the probability of getting caught there is small. In fact, the WKB approximation is sometimes *derived* by starting with this "semi-classical" observation, instead of by dropping the A'' term in the differential equation. The latter approach is cleaner mathematically, but the former offers a more plausible physical rationale.

Example 8.1 Potential well with two vertical walls. Suppose we have an infinite square well with a bumpy bottom (Figure 8.2):

$$V(x) = \begin{cases} \text{some specified function}, & \text{if } 0 < x < a, \\ \infty, & \text{otherwise}. \end{cases} \qquad [8.12]$$

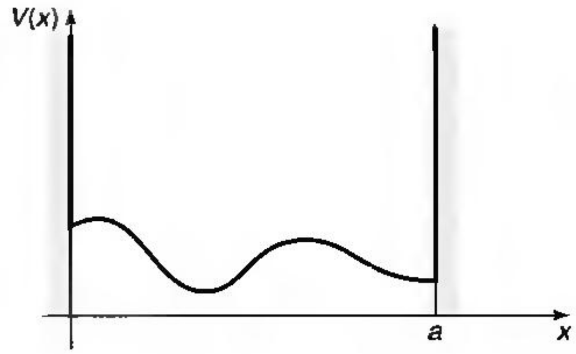

FIGURE 8.2: Infinite square well with a bumpy bottom.

Inside the well (assuming $E > V(x)$ throughout) we have

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}}\left[C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)}\right],$$

or, more conveniently,

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}}\left[C_1 \sin\phi(x) + C_2 \cos\phi(x)\right], \qquad [8.13]$$

where (exploiting the freedom noted earlier to impose a convenient lower limit on the integral)

$$\phi(x) = \frac{1}{\hbar}\int_0^x p(x')\,dx'. \qquad [8.14]$$

Now $\psi(x)$ must go to zero at $x = 0$, and therefore (since $\phi(0) = 0$) $C_2 = 0$. Also, $\psi(x)$ goes to zero at $x = a$, so

$$\phi(a) = n\pi \quad (n = 1, 2, 3, \ldots). \qquad [8.15]$$

Conclusion:

$$\boxed{\int_0^a p(x)\,dx = n\pi\hbar.} \qquad [8.16]$$

This quantization condition determines the (approximate) allowed energies.

For instance, if the well has a *flat* bottom ($V(x) = 0$), then $p(x) = \sqrt{2mE}$ (a constant), and Equation 8.16 says $pa = n\pi\hbar$, or

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},$$

which is the old formula for the energy levels of the infinite square well (Equation 2.27). In this case the WKB approximation yields the *exact* answer (the amplitude of the true wave function is *constant*, so dropping A'' cost us nothing).

***Problem 8.1** Use the WKB approximation to find the allowed energies (E_n) of an infinite square well with a "shelf," of height V_0 extending half-way across (Figure 6.3):

$$V(x) = \begin{cases} V_0, & \text{if } 0 < x < a/2, \\ 0, & \text{if } a/2 < x < a, \\ \infty, & \text{otherwise.} \end{cases}$$

Express your answer in terms of V_0 and $E_n^0 \equiv (n\pi\hbar)^2/2ma^2$ (the nth allowed energy for the infinite square well with *no* shelf). Assume that $E_1^0 > V_0$, but do *not* assume that $E_n \gg V_0$. Compare your result with what we got in Example 6.1 using first-order perturbation theory. Note that they are in agreement if either V_0 is very small (the perturbation theory regime) or n is very large (the WKB—semi-classical—regime).

****Problem 8.2** An illuminating alternative derivation of the WKB formula (Equation 8.10) is based on an expansion in powers of $\hbar$. Motivated by the free-particle wave function, $\psi = A\exp(\pm ipx/\hbar)$, we write

$$\psi(x) = e^{if(x)/\hbar},$$

where $f(x)$ is some *complex* function. (Note that there is no loss of generality here—*any* nonzero function can be written in this way.)

(a) Put this into Schrödinger's equation (in the form of Equation 8.1), and show that

$$i\hbar f'' - (f')^2 + p^2 = 0.$$

(b) Write $f(x)$ as a power series in $\hbar$:

$$f(x) = f_0(x) + \hbar f_1(x) + \hbar^2 f_2(x) + \cdots,$$

and, collecting like powers of $\hbar$, show that

$$(f_0')^2 = p^2, \quad if_0'' = 2f_0'f_1', \quad if_1'' = 2f_0'f_2' + (f_1')^2, \quad \text{etc.}$$

(c) Solve for $f_0(x)$ and $f_1(x)$, and show that—to first order in $\hbar$—you recover Equation 8.10.

Note: The logarithm of a negative number is defined by $\ln(-z) = \ln(z) + in\pi$, where n is an odd integer. If this formula is new to you, try exponentiating both sides, and you'll see where it comes from.

8.2 TUNNELING

So far, I have assumed that $E > V$, so $p(x)$ is real. But we can easily write down the corresponding result in the *non*classical region ($E < V$)—it's the same as before (Equation 8.10), only now $p(x)$ is *imaginary*:[2]

$$\psi(x) \cong \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar} \int |p(x)| dx}. \tag{8.17}$$

Consider, for example, the problem of scattering from a rectangular barrier with a bumpy top (Figure 8.3). To the left of the barrier ($x < 0$),

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \tag{8.18}$$

where A is the incident amplitude, B is the reflected amplitude, and $k \equiv \sqrt{2mE}/\hbar$ (see Section 2.5). To the right of the barrier ($x > a$),

$$\psi(x) = Fe^{ikx}; \tag{8.19}$$

F is the transmitted amplitude, and the transmission probability is

$$T = \frac{|F|^2}{|A|^2}. \tag{8.20}$$

In the tunneling region ($0 \leq x \leq a$), the WKB approximation gives

$$\psi(x) \cong \frac{C}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar} \int_0^x |p(x')| dx'} + \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar} \int_0^x |p(x')| dx'}. \tag{8.21}$$

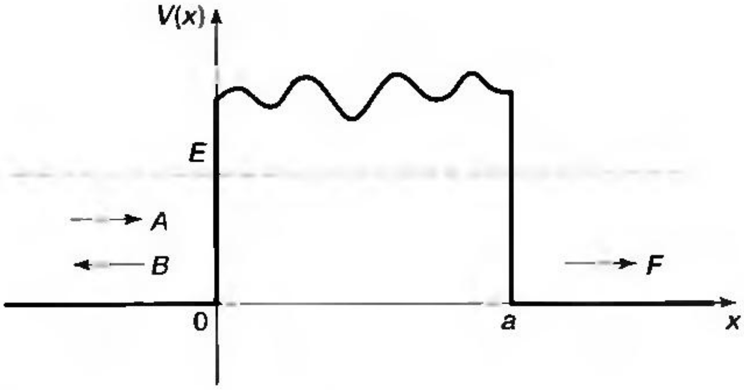

FIGURE 8.3: Scattering from a rectangular barrier with a bumpy top.

[2] In this case the wave function is *real*, and the analogs to Equations 8.6 and 8.7 do not follow *necessarily* from Equation 8.5, although they are still *sufficient*. If this bothers you, study the alternative derivation in Problem 8.2.

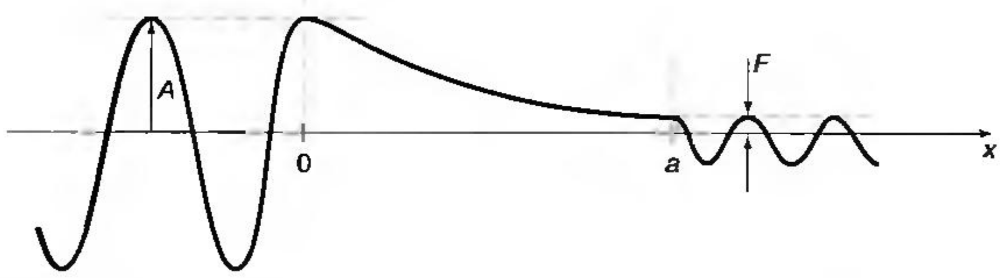

FIGURE 8.4: Qualitative structure of the wave function, for scattering from a high, broad barrier.

If the barrier is very high and/or very wide (which is to say, if the probability of tunneling is small), then the coefficient of the exponentially *increasing* term (C) must be small (in fact, it would be *zero* if the barrier were *infinitely* broad), and the wave function looks something like[3] Figure 8.4. The relative amplitudes of the incident and transmitted waves are determined essentially by the total decrease of the exponential over the nonclassical region:

$$\frac{|F|}{|A|} \sim e^{-\frac{1}{\hbar}\int_0^a |p(x')|\,dx'},$$

so that

$$T \cong e^{-2\gamma}, \quad \text{with } \gamma \equiv \frac{1}{\hbar}\int_0^a |p(x)|\,dx. \qquad [8.22]$$

Example 8.2 Gamow's theory of alpha decay.[4] In 1928, George Gamow (and, independently, Condon and Gurney) used Equation 8.22 to provide the first successful explanation of alpha decay (the spontaneous emission of an alpha-particle—two protons and two neutrons—by certain radioactive nuclei).[5] Since the alpha particle carries a positive charge ($2e$), it will be electrically repelled by the leftover nucleus (charge Ze), as soon as it gets far enough away to escape the nuclear binding force. But first it has to negotiate a potential barrier that was already known (in the case of uranium) to be more than twice the energy of the emitted alpha particle. Gamow approximated the potential energy by a finite square well (representing the attractive nuclear force), extending out to r_1 (the radius of the nucleus), joined

[3]This heuristic argument can be made more rigorous—see Problem 8.10.

[4]For a more complete discussion, and alternative formulations, see Barry R. Holstein, *Am. J. Phys.* **64**, 1061 (1996).

[5]For an interesting brief history see Eugen Merzbacher, "The Early History of Quantum Tunneling," *Physics Today*, August 2002, p. 44.

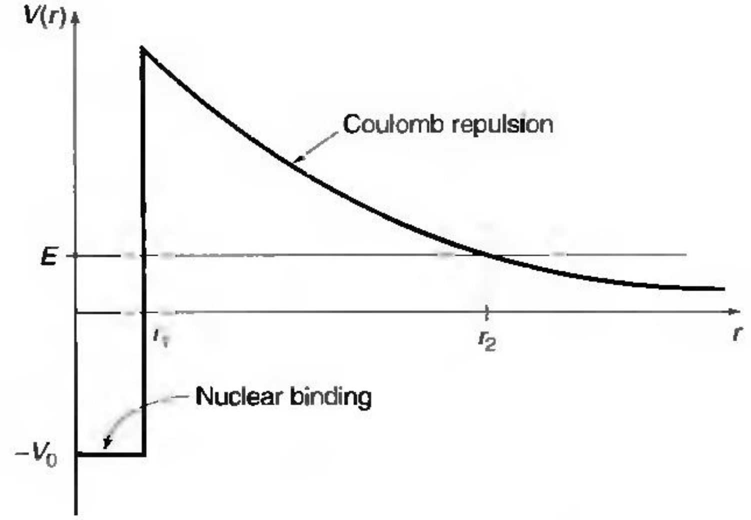

FIGURE 8.5: Gamow's model for the potential energy of an alpha particle in a radioactive nucleus.

to a repulsive coulombic tail (Figure 8.5), and identified the escape mechanism as quantum tunneling (this was, by the way, the first time that quantum mechanics had been applied to nuclear physics).

If E is the energy of the emitted alpha particle, the outer turning point (r_2) is determined by

$$\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r_2} = E. \qquad [8.23]$$

The exponent γ (Equation 8.22) is evidently[6]

$$\gamma = \frac{1}{\hbar}\int_{r_1}^{r_2}\sqrt{2m\left(\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r} - E\right)}\,dr = \frac{\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{r_2}{r} - 1}\,dr.$$

The integral can be done by substitution (let $r \equiv r_2 \sin^2 u$), and the result is

$$\gamma = \frac{\sqrt{2mE}}{\hbar}\left[r_2\left(\frac{\pi}{2} - \sin^{-1}\sqrt{\frac{r_1}{r_2}}\right) - \sqrt{r_1(r_2 - r_1)}\right]. \qquad [8.24]$$

Typically, $r_1 \ll r_2$, and we can simplify this result using the small angle approximation ($\sin\epsilon \cong \epsilon$):

$$\gamma \cong \frac{\sqrt{2mE}}{\hbar}\left[\frac{\pi}{2}r_2 - 2\sqrt{r_1 r_2}\right] = K_1\frac{Z}{\sqrt{E}} - K_2\sqrt{Zr_1}. \qquad [8.25]$$

[6]In this case the potential does not drop to zero on the left side of the barrier (moreover, this is really a three-dimensional problem), but the essential idea, contained in Equation 8.22, is all we really need.

where

$$K_1 \equiv \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{\pi\sqrt{2m}}{\hbar} = 1.980 \text{ MeV}^{1/2}, \quad [8.26]$$

and

$$K_2 \equiv \left(\frac{e^2}{4\pi\epsilon_0}\right)^{1/2}\frac{4\sqrt{m}}{\hbar} = 1.485 \text{ fm}^{-1/2}. \quad [8.27]$$

[One fermi (fm) is 10^{-15} m, which is about the size of a typical nucleus.]

If we imagine the alpha particle rattling around inside the nucleus, with an average velocity v, the average time between "collisions" with the "wall" is about $2r_1/v$, and hence the *frequency* of collisions is $v/2r_1$. The probability of escape at each collision is $e^{-2\gamma}$, so the probability of emission, per unit time, is $(v/2r_1)e^{-2\gamma}$, and hence the **lifetime** of the parent nucleus is about

$$\tau = \frac{2r_1}{v}e^{2\gamma}. \quad [8.28]$$

Unfortunately, we don't know v—but it hardly matters, for the exponential factor varies over a *fantastic* range (twenty-five orders of magnitude), as we go from one radioactive nucleus to another; relative to this the variation in v is pretty insignificant. In particular, if you plot the *logarithm* of the experimentally measured lifetime against $1/\sqrt{E}$, the result is a beautiful straight line (Figure 8.6),[7] just as you would expect from Equations 8.25 and 8.28.

∗Problem 8.3 Use Equation 8.22 to calculate the approximate transmission probability for a particle of energy E that encounters a finite square barrier of height $V_0 > E$ and width $2a$. Compare your answer with the exact result (Problem 2.33), to which it should reduce in the WKB regime $T \ll 1$.

∗∗Problem 8.4 Calculate the lifetimes of U^{238} and Po^{212}, using Equations 8.25 and 8.28. *Hint:* The density of nuclear matter is relatively constant (i.e., the same for all nuclei), so $(r_1)^3$ is proportional to A (the number of neutrons plus protons). Empirically,

$$r_1 \cong (1.07 \text{ fm})A^{1/3}. \quad [8.29]$$

[7] From David Park, *Introduction to the Quantum Theory*, 3rd ed., McGraw-Hill (1992); it was adapted from I. Perlman and J. O. Rasmussen, "Alpha Radioactivity," *Encyclopedia of Physics*, Vol. **42**, Springer (1957). This material is reproduced with permission of The McGraw-Hill Companies.

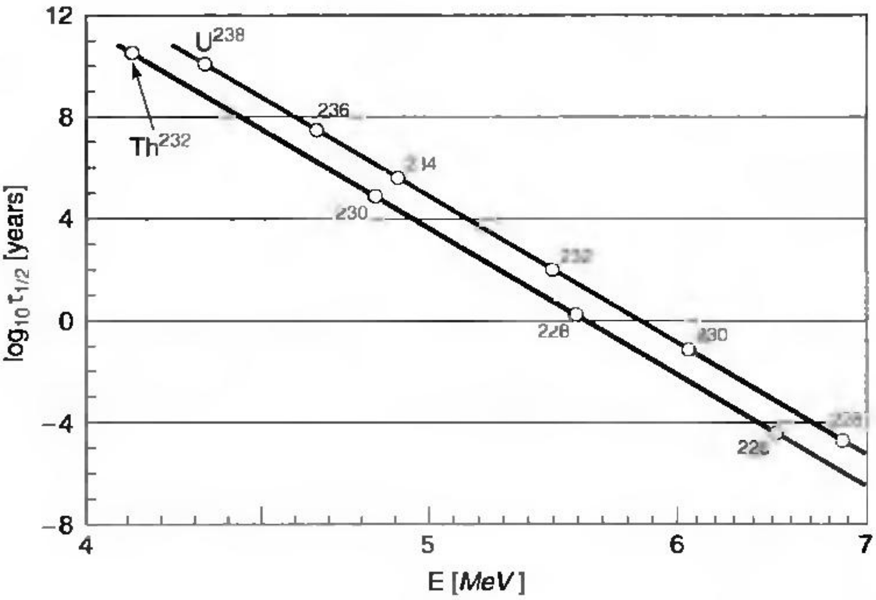

FIGURE 8.6: Graph of the logarithm of the lifetime versus $1/\sqrt{E}$ (where E is the energy of the emitted alpha particle), for uranium and thorium.

The energy of the emitted alpha particle can be deduced by using Einstein's formula ($E = mc^2$):

$$E = m_p c^2 - m_d c^2 - m_\alpha c^2. \qquad [8.30]$$

where m_p is the mass of the parent nucleus, m_d is the mass of the daughter nucleus, and m_α is the mass of the alpha particle (which is to say, the He^4 nucleus). To figure out what the daughter nucleus is, note that the alpha particle carries off two protons and two neutrons, so Z decreases by 2 and A by 4. Look up the relevant nuclear masses. To estimate v, use $E = (1/2)m_\alpha v^2$; this ignores the (negative) potential energy inside the nucleus, and surely *underestimates* v, but it's about the best we can do at this stage. Incidentally, the experimental lifetimes are 6×10^9 yrs and 0.5 μs, respectively.

[redacted]