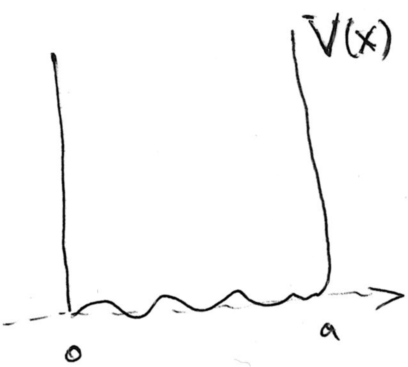
Bohr - Sommerfeld quantization rules

In the previous lecture we have obtained that up to first order in $\hbar$ the semiclassical approximation takes the following form

$$\psi \approx \frac{1}{\sqrt{p(x)}}\left[C_+ e^{\frac{i}{\hbar}\int p(x)dx} + C_- e^{-\frac{i}{\hbar}\int p(x)dx}\right]$$

where $p(x) = \sqrt{2m(E - V(x))}$

Now let us apply this formula to the case of a potential with two infinite (vertical) walls. We can rewrite $\psi(x)$ as



$$\psi(x) = \frac{1}{\sqrt{p(x)}}\left[C \sin\phi(x) + D\cos\phi(x)\right]$$

with $\phi(x) = \frac{1}{\hbar}\int_0^x p(x')\,dx'$

Since the potential becomes infinite at $x=0$ the boundary condition is $\psi(0)=0$. Now since $\phi(0)=0$ D must be equal to zero. Also $\psi(x)$ goes to zero at $x=a$. Then

$$\phi(a) = n\pi \qquad n = 1,2,3,\dots$$

($n=0$ excluded, because in that case $\psi = 0$)

Hence we conclude that

$$\int_0^a p(x)\,dx = n\pi\hbar \longrightarrow$$ this condition determines energy

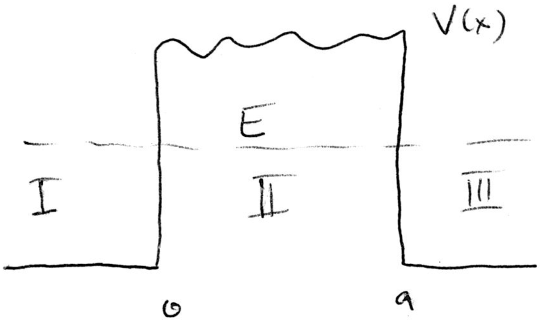
If we consider the infinite square well (which we know how to solve exactly) then

$$n\pi\hbar = \int_0^a p(x)dx = \int_0^a \sqrt{2mE}\,dx = \sqrt{2mE}\,a \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

In this particular case the WKB approximation recovers the exact formula for E_n.

Barrier tunneling in WKB approximation

We can also consider scattering (i.e. when $E < V$) and transmission through a potential barrier.



In region I:

$$\psi = Ae^{ikx} + Be^{-ikx} \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

In region III

$$\psi = Fe^{ikx}$$

As we know the transmission coefficient is defined as

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

In region II we can use the WKB approximation

$$\psi = \frac{C}{\sqrt{\varkappa(x)}} e^{\int_0^x \varkappa(x')dx'} + \frac{D}{\sqrt{\varkappa(x)}} e^{-\int_0^x \varkappa(x')dx'}$$

where $\varkappa(x) = \frac{1}{\hbar}\sqrt{2m(V(x)-E)} = \frac{|p(x)|}{\hbar}$

If we assume that the barrier is wide and high so that the tunneling probability is small then the term $\frac{C}{\sqrt{\varkappa(x)}} e^{\int_0^x \varkappa(x')dx'}$ must also be small (because ψ must decay). The relative amplitudes of the incident and transmitted waves are determined by the total decrease of the exponential over the nonclassical region

$$\frac{|F|}{|A|} \sim e^{-\int_0^a \varkappa(x')dx}$$

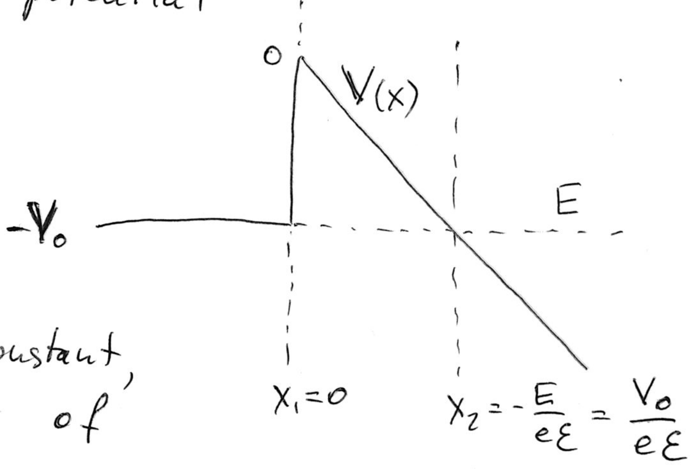
and

$$T = e^{-2\gamma} \qquad \gamma = \int_0^a \varkappa(x')\,dx$$

Cold emission of electrons from metal

As an application of the WKB approximation let us consider the phenomenon of cold emission of electrons from metal when it is placed in an external electric field. We can model an electron as beign trapped inside the metal by the potential

$$V(x) = \begin{cases} -V_0 & , x<0 \\ -e\mathcal{E}x & , x \geq 0 \end{cases}$$



where V_0 is a positive constant, and $\mathcal{E}$ is the magnitude of the external electric field.

The tunneling probability in the WKB approximation is

$$T = \exp[-2\gamma] \qquad \gamma = \frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V(x)-E)}\, dx$$

The integral is easy to evaluate:

$$\int_{x_1}^{x_2} \sqrt{2m(V(x)-E)}\, dx = \sqrt{2m}\int_0^{\frac{|E|}{e\mathcal{E}}} \sqrt{-E-e\mathcal{E}x}\, dx = \sqrt{2m}\,|E|^{1/2}\int_0^{\frac{|E|}{e\mathcal{E}}} \left[1-\frac{e\mathcal{E}x}{|E|}\right]^{1/2} dx =$$

$$= \sqrt{2m}\,|E|^{1/2} \underbrace{\int_0^1 [1-y]^{1/2}\, dy}_{2/3} = \frac{2}{3}\frac{\sqrt{2m}\,|E|^{3/2}}{e\mathcal{E}}$$

Then the tunneling probability becomes

$$T = \exp\left[-\frac{4}{3}\frac{\sqrt{2m}\,|E|^{3/2}}{3e\mathcal{E}\hbar}\right]$$

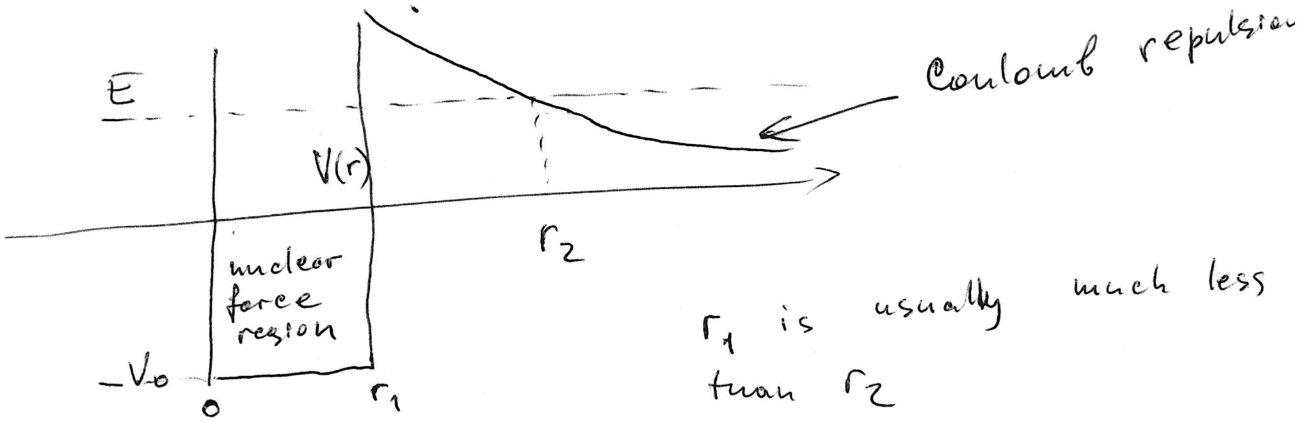
In the ground state for an electron in the metal $E=-V_0$, so

$$T = \exp\left[-\frac{4}{3}\frac{\sqrt{2m}\,V_0^{3/2}}{e\mathcal{E}\hbar}\right]$$

— Fowler-Nordheim formula

Gamow's theory of alpha decay

The WKB approximation in the context of barrier tunneling can be used to describe the spontaneous emission of α-particles by some radioactive nuclei.



r_1 is usually much less than r_2

Turning point are r_1 and r_2

$$\underbrace{\frac{1}{4\pi\varepsilon_0}\frac{2Ze^2}{r_2}}_{\text{Coulomb repulsion of a positively charged } \alpha\text{-particle from the rest of the nucleus at large distances}} = E$$

(the charge of the alpha particle is $2e$)

$$\gamma = \int_{r_1}^{r_2} \varkappa(r)\, dr = \frac{\sqrt{2m}}{\hbar}\int_{r_1}^{r_2}\sqrt{V(r)-E}\, dr = \frac{\sqrt{2m}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{2Ze^2}{4\pi\varepsilon_0 r}-E}\, dr$$

$$= \frac{\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{r_2}{r}-1}\, dr$$

Here we use the integral taken from a table of integrals

$$\int\sqrt{\frac{a}{x}-1}\, dx = \sqrt{\frac{a}{x}-1}\, x - \frac{a}{2}\arctan\left[\frac{\sqrt{\frac{a}{x}-1}}{2}\frac{2x-a}{x-a}\right]$$

So

$$\gamma = \frac{\sqrt{2mE}}{\hbar}\left(\sqrt{\frac{r_2}{r}-1}\, r - \frac{r_2}{2}\arctan\left[\frac{\sqrt{\frac{r_2}{r}-1}}{2}\frac{2r-r_2}{r-r_2}\right]\right)\Bigg|_{r_1}^{r_2} =$$

$$= \frac{\sqrt{2mE}}{\hbar}\left(-\sqrt{(r_2-r_1)r_1} + \frac{r_2}{2}\arctan\left[\frac{1}{2}\frac{r_2-2r_1}{\sqrt{(r_2-r_1)r_1}}\right] + \frac{\pi r_2}{4}\right)$$

Note that $\arctan(x) \underset{x\to\infty}{\approx} \frac{\pi}{2} - \frac{1}{x} + \frac{1}{3x^3} + \ldots$

If $r_2 >> r_1$ then $\gamma = \frac{\sqrt{2mE}}{\hbar}\left(-\sqrt{r_2 r_1} + \frac{r_2}{2}\left(\frac{\pi}{2} - 2\sqrt{\frac{r_1}{r_2}}\right) + \frac{\pi r_2}{4}\right) =$

$= \frac{\sqrt{2mE}}{\hbar}\left[\frac{\pi}{2} r_2 - 2\sqrt{r_1 r_2}\right]$

It can also be written as

$\gamma = k_1 \frac{Z}{\sqrt{E}} - k_2\sqrt{Z r_1}$ where $k_1 = \left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{\pi\sqrt{2m}}{\hbar} \approx 1.98 \text{ MeV}^{1/2}$

$k_2 = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^{1/2}\frac{4\sqrt{m}}{\hbar} \approx 1.485 \text{ fm}^{-1/2}$

Each time between collisions with the walls the alpha-particle travels the distance $2r_1$ (nuclear diameter). The frequency of the collision with the barrier is then $\frac{v}{2r_1}$, where v is the particle's velocity. The probability of emission per unit time is $\beta = \frac{v}{2r_1}e^{-2\gamma}$. The number of nuclei that decay in time dt is

$$dN = -\beta N dt$$

Which gives the following formula for the number of non-decayed nuclei:

$$N(t) = N_0 e^{-\beta t}$$

The lifetime of the nucleus is then

$$\tau = \frac{1}{\beta} = \frac{2r_1}{v}e^{2\gamma}$$