

Electronic Properties of the Materials: Computational Approach
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Lecture: 10
The WKB Approximation Method (Part 2)

Hello friends in the last lecture we learned about WKB approximation and used it to solve a problem on particle in a box having some finite potential inside the box. In this lecture we are going to continue our discussion on WKB approximation and apply to solve a problem on quantum tunnelling.

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Constant potential barrier

TISE:-

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

$$\Rightarrow \frac{d^2\psi}{dx^2} = \frac{2m(V-E)}{\hbar^2} \psi = \alpha^2 \psi$$

$$\alpha = \sqrt{2m(V-E)}$$

$$\Rightarrow \psi(x) = A e^{\pm \alpha x / \hbar}, \quad \frac{\alpha \hbar}{\hbar} = \gamma$$

$$= A e^{\pm \gamma x}$$

• Particle moving through a region of constant potential and $E < V$ (non-classical region)

In the last lecture we have considered a case where energy of the particle is more than the potential barrier. In this lecture we consider a case where energy of the particle is less than the potential barrier. Note that classically the particle is going to be reflected from this point because of the potential barrier. However we know that a quantum particle can tunnel and penetrate in a region forbidden classically.

We write the time independent Schrodinger equation as $-\hbar^2 \frac{d^2\psi}{dx^2} + V\psi = E\psi$ and then we just rearrange the equation as $\frac{d^2\psi}{dx^2} = \frac{2m(V-E)}{\hbar^2} \psi$ and we write it as $q^2 \psi$ where q is given by square root of $2m(V-E)$ and the solution of this equation

is given by $\psi(x)$ is equal to $A e^{\pm \gamma x}$ divided by \hbar . And we just write q by \hbar equal to γ such that the solution is $A e^{\pm \gamma x}$.

Note that since q is real the wave function is exponential with fixed q and A and as we have already learned the wave function is given by $\psi(x)$ is equal to $A e^{\pm \gamma x}$ and γ is equal to $1/\hbar$ times q . Now this is for the case of a constant potential. What happens if V is not a constant and very slowly in space that is V is a function of x this is what we are going to learn in the next slide.

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- You can think of "imaginary momentum", such that $|p(x)| = q(x)$
- WKB approximation: still we get an exponential wave function
- $\psi(x) = A(x)e^{\pm \gamma(x)}$, $\psi(x)$: real function
- $A(x) = \frac{C}{\sqrt{q(x)}}$ ←
- $\gamma(x) = \frac{1}{\hbar} \int q(x') dx'$ ←
- Probability of finding the "particle" in space: $|\psi(x)|^2 = \frac{|C|^2}{q(x)}$
- Probability of finding a "particle" at a point is inversely proportional to $q(x)$ ←

Momentum: $p = \sqrt{2m(E-V)}$
 $V > E$, $p \rightarrow$ imaginary

Since the potential energy is varying slowly in space q is not a constant but this also varies slowly in space. Momentum is defined as square root of difference between total energy and potential energy that is momentum p is equal to square root of $2mE - V$. In this case we have V is greater than E thus is imaginary. Thus we can correlate q with some imaginary momentum such that the magnitude of the imaginary momentum is equal to q of x .

Similar to the case of constant q WKB approximation tells us that we still get an exponential wave function $\psi(x)$ is equal to $A(x)e^{\pm \gamma(x)}$. But now both A and γ changes slowly with x γ is given by the integral of q and A of x is equal to C divided by square root of q of x . Probability of finding the particle in space is given by mod of $\psi(x)$ square is equal to C^2 divided by $q(x)$ thus probability of finding a particle at a point is inversely proportional to q of x .

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Constant potential	Slowly varying potential
<ul style="list-style-type: none"> • TISE: $\frac{d^2\psi}{dx^2} = \frac{q^2}{\hbar^2}\psi; q^2 > 0$ • $q = \sqrt{2m(V - E)}$ • Wave function: $\psi(x) = Ae^{\pm\gamma x}$ • $\psi(x)$ is a real function • A constant • $\gamma = \frac{1}{\hbar}qx$ 	<ul style="list-style-type: none"> • $\frac{d^2\psi}{dx^2} = \frac{q^2}{\hbar^2}\psi; q^2 > 0$ • $q(x) = \sqrt{2m[V(x) - E]}$ • $\psi(x) = A(x)e^{\pm\gamma(x)}$ • $\psi(x)$ is a real function • $A(x) = \frac{C}{\sqrt{q(x)}}$ • $\gamma(x) = \frac{1}{\hbar} \int^x q(x')dx'$

Let us go back to tunneling problem and solve it using WKB approximation

Before proceeding further let me show the case of constant and slowly varying potential side by side time independent Schrodinger equation is given by $\frac{d^2\psi}{dx^2} = \frac{q^2}{\hbar^2}\psi$ where q^2 is greater than zero, q is constant in case of a constant potential and it varies slowly in space. Wave function $\psi(x)$ is exponential in both the cases and it is a real function.

However in case of a slowly varying potential q of x also varies slowly in space and given by C divided by square root of q of x and γ of x can be obtained by integrating q of x . Now let us go back to the tunnelling problem and we solve it using WKB approximation.

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- Left of the barrier: $\psi_I(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$
- Right of the barrier: $\psi_{III}(x) = Fe^{ipx/\hbar}$
- $p = \sqrt{2mE}$
- Inside the barrier (WKB): $\psi_{II}(x) = \frac{C}{\sqrt{q(x)}}e^{\gamma(x)} + \frac{D}{\sqrt{q(x)}}e^{-\gamma(x)}$
- $\gamma(x) = \frac{1}{\hbar} \int_0^x q(x')dx'$
- $q(x) = \sqrt{2m(V(x) - E)}$
- If a is very large, we can approximate: $\psi_{II}(x) \approx \frac{D}{\sqrt{q(x)}}e^{-\gamma(x)}$
 - ▶ In the limit $a \rightarrow \infty$, this is the exact solution
 - ▶ Because $e^{\gamma(x)}$ blows up as $x \rightarrow \infty$, so $C = 0$
- Same approximation works if $V(x) \gg E$

We have a potential barrier from x equal to 0 to x equal to a shown by the blue line note that it is not a constant but changes continuously in space potential energy is 0 in the left hand side

and in the right hand side of the barrier. Wave function is oscillatory in the left hand side of the barrier the incident wave is travelling from the left to the right and the reflected wave is travelling from the right to the left.

And the reflection is taking place because of the potential barrier. Wave function is oscillatory in the right hand side of the barrier also and in this case the transmitted wave is travelling from the left to the right. The transmitted wave has smaller amplitude compared to the incident wave. For example you see here that incident wave has a very large amplitude whereas the transmitted wave has a relatively smaller amplitude.

We have to find the ratio of the amplitude of the transmitted and incident wave which gives us the transmission coefficient. Inside the barrier the wave function is exponential and using WKB approximation we can write it as C divided by square root of q times $e^{-\gamma(x)}$ divided by square root of q times $e^{\gamma(x)}$ can be calculated from the integral of the q and q is defined as square root of $2m(V(x) - E)$.

If a is very large we can approximate ψ_{II} as b divided by square root of q times $e^{-\gamma(x)}$ that means we drop the first term. In the limit a going to infinity this is the exact solution because in this case if $e^{-\gamma(x)}$ blows up at x goes to infinity. So, we have to make C is equals to zero such that the first part is zero and we are left only with the second part. The same approximation works if $V(x)$ is much larger than the value of the energy.

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right of the barrier:
 $\psi_{III}(x) = F e^{ipx/\hbar}$
 $p = \sqrt{2mE}$

- Inside the barrier (large a): $\psi_{II}(x) \approx \frac{D}{\sqrt{q(x)}} e^{-\gamma(x)}$
- $\gamma(x) = \frac{1}{\hbar} \int_0^x q(x') dx'$, and $q(x) = \sqrt{2m(V(x) - E)}$
- $\psi_{II}(0) = \frac{D}{\sqrt{q(0)}}$, and $\psi_{II}(a) = \frac{D}{\sqrt{q(a)}} e^{-\gamma(a)}$
- Decrease of ψ_{II} from left to right: $\frac{\psi_{II}(a)}{\psi_{II}(0)} = \sqrt{\frac{q(0)}{q(a)}} e^{-\gamma(a)}$
- Relative amplitude of incident & transmitted: $\frac{|F|}{|A|} \approx \sqrt{\frac{q(0)}{q(a)}} e^{-\gamma(a)}$
 - ▶ Constant potential: $\frac{q(0)}{q(a)} = 1$
 - ▶ Slowly varying potential: $\frac{q(0)}{q(a)} \approx 1$

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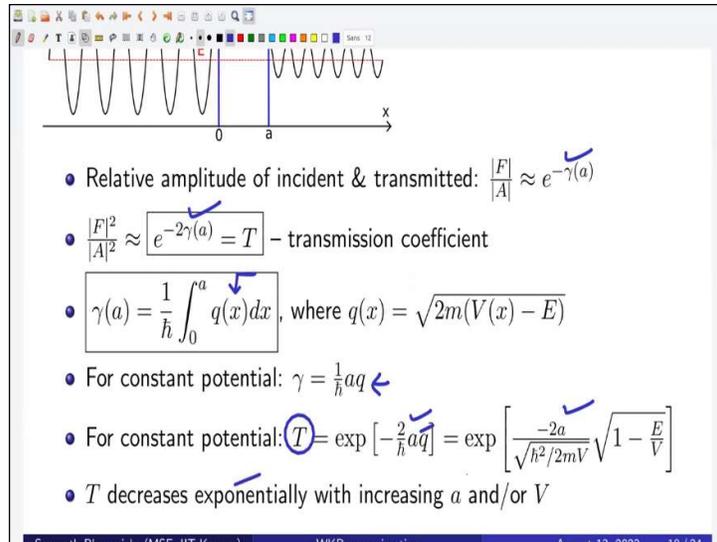
Thus left of the barrier we know the exact wave function given by $\psi_1(x)$ is equal to $A e^{i p x / \hbar} + B e^{-i x / \hbar}$. Similarly in the right of the barrier we know now a function exactly $\psi_3(x)$ is equal to $f e^{i dx / \hbar}$. Since V is equal to 0 it is equal to momentum and given by square root of $2 m E$ inside the barrier we write the wave function using WKB approximation and in the limit of large a the wave function is $\psi_2(x)$ is equal to $D \sqrt{q} e^{-\int q dx}$ is given by the integral of q .

Now let us try to find ψ_2 at x equal to 0 and at x equal to a . So, to get ψ_2 at x equal to 0 we have to evaluate this integral $\int_0^0 q dx$ and you see that in this case since the upper limit of the integral is equal to 0 \int_0^0 has to be equal to 0 in that case $\psi_2(0)$ is equal to $b / \sqrt{q_0}$ and at x equal to a we have $\int_0^a q dx$ and in this case the upper limit of the integral is a .

And thus $\psi_2(a)$ is equal to $d / \sqrt{q_a} e^{-\int_0^a q dx}$. Now the wave function decreases in the classically forbidden region and the decrease of ψ_2 from the left to the right is given by $\psi_2(a) / \psi_2(0)$ and this is equal to $\sqrt{q_0} / \sqrt{q_a} e^{-\int_0^a q dx}$. By calculating the decrease of ψ_2 in the non classical region we get the relative amplitude of the incident and transmitted wave that is $|f| / |b|$ is given by the decrease of ψ_2 in the non classical region.

Note that if we have a constant potential in that case the ratio of q_0 / q_a is equal to 1. Now in case of a slowly varying potential also we can just approximate q_0 by q_a to be a number which is of the order of 1 and we can ignore it.

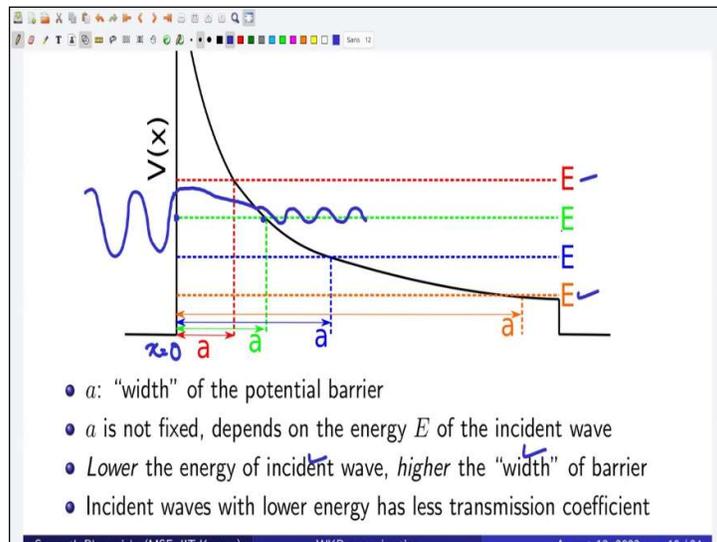
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Thus relative amplitude of incident and transmitted wave is given by $e^{-\gamma a}$. Now if we take a square of this that gives us the transmission coefficient. Note that γa can be calculated by integrating q of x where q of x is given by square root of $2m(V - E)$. Note that for a constant potential γ is just $1/\hbar$ times a times q and thus for a constant potential p is equal to $e^{-2/\hbar a q}$.

And we can put the value of q in this equation and we can rewrite the transmission coefficient in this form. Thus we find that the transmission coefficient p decreases exponentially with increasing a and oblique odd with increasing V .

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Let us take a case where V of x is inversely proportional to x as shown here. Now the quantum particle hits the barrier at x equal to 0 and then it exits the variable x equal to a . Distance that

the particle needs to cross before it can escape the potential barrier depends on the energy thus the width of the barrier is not fixed but it depends on the value of energy E . Lower the energy of the incident wave higher is the width of the area.

For example in this case for the orange line the energy is minimum and width of the potential barrier a is maximum. On the other hand for the red line the energy is maximum and width of the potential barrier is minimum. Since transmission coefficient decays exponentially with the barrier width incident waves with lower energy has less transmission coefficient. let us write a code to calculate this.

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Let me first explain the code the potential is taken to be $1/(1+x)$. The incident wave hits the barrier at x equal to 0 and escapes at x equal to a . Now value of a depends on the value of energy of the incident wave. Now at the point where it escapes the potential barrier the value of energy is equals to value of the potential energy thus in this equation if we just put e is equals to $1/(1+a)$.

And then from this we can estimate the value of a this is done in this step here. Then we need to find the transmission coefficient transmission coefficient is given by $e^{-2 \times \text{gamma of } a}$ where $\text{gamma of } a$ is given by the integral of q . In the code we define q here and then the numerical integral to calculate $\text{gamma of } a$ is done over here and finally the user defined function that calculates the value of gamma returns the value of gamma .

In this step the transmission coefficient is calculated using a for loop we are using a for loop because we want to calculate the transmission coefficient for different values of energy. And energy value is varied from 0.01 to 0.1 we call the function to calculate gamma in this step and using that value we are calculating the value of the transmission coefficient for different values of energy finally we plot the results in this step.

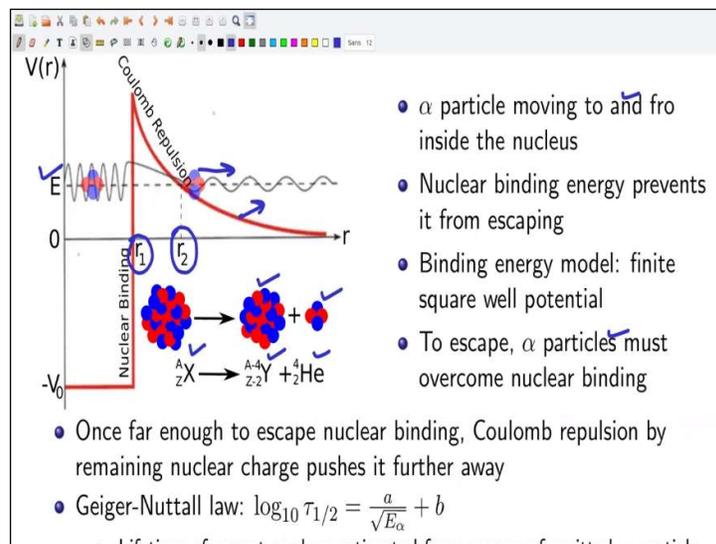
Let us take a closer look at the code and then run it to generate the plot of transmission coefficient as a function of energy of the incident wave. This is where we define the energy range for the incident wave varying between 0.01 to 0.1. Then we have one user defined function to calculate gamma first we find the width of the potential in this step then we define the potential function V then we define the function q and finally we integrate q to get the value of gamma .

The function returns the value of gamma for some given energy. Here we have a for loop which calls the user defined function to calculate gamma and find the transmission coefficient for different energy of incident wave. Finally we plot the transmission coefficient as a function of the energy let us run the code. This is the plot of transmission coefficient as a function of energy generated by our code.

Note that both x and y axis is in log scale energy of the incident wave changes just by one order of magnitude. However the transmission coefficient changes by almost 14 orders of magnitude.

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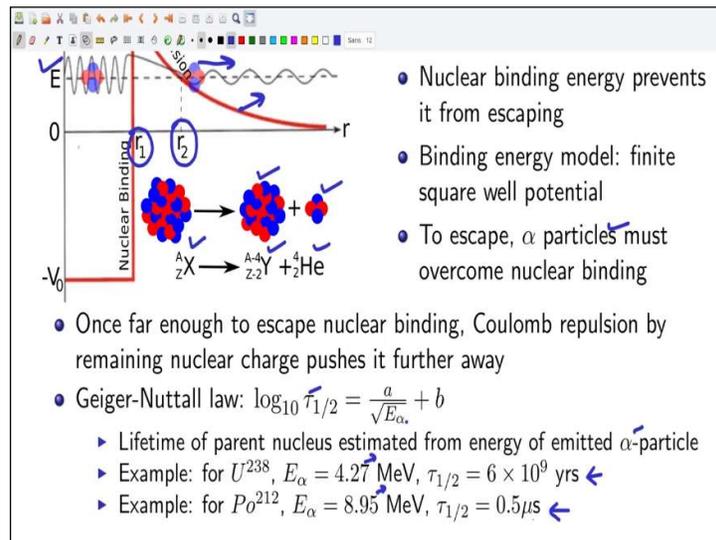
The type of potential we have chosen for our code is very similar to what we get in case of Gamow's theory of alpha decay. In case of alpha decay the parent nucleus x emits an alpha particle and it is converted to some other nucleus y . Before the decay the alpha particle moves to and flow inside the nucleus and energy of the alpha particle is e as shown in this diagram. Strong nuclear binding prevents the particle from escaping the nucleus.

A finite square well potential is the simplest possible model for nuclear binding. The final barrier which is typically having a height of more than twice the energy of the alpha particle prevents the alpha particle from escaping the nucleus. Note that we cannot take some infinite square well potential because in that case the alpha particle will never be able to escape. To escape the alpha particle must tunnel through the barrier.

Once far enough from the nucleus Coulomb repulsion by remaining nuclear charges pushes it further away and alpha particle finally escapes. If we assume the square well potential barrier is at r_1 the particle has to channel all the way to r_2 and then we see that the Coulomb repulsion will push it further away. Note that the coulomb repulsion is repulsive because the alpha particle is positively charged and the remaining nucleus is also positively charged.

Note the similarity of potential profile shown by the red line in this picture between Gamow's theory of alpha decay and what we did with the code for tunnelling through potential barrier.

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Geiger-Nuttall law relates the lifetime of the parent nucleus with the energy of the emitted alpha particle which can be experimentally measured. The relation is log of lifetime is equals to a divided by square root of E alpha + b where E alpha is the energy of the alpha particle. Thus one can estimate the lifetime of current nucleus from energy of the emitted alpha particle. For example for uranium 238 the energy of the emitter alpha particle is 4.27 MeV where 1 MeV is equals to 10 power 6 electron volt.

On the other hand for polonium 212 the e alpha is 8.95 MeV. Note that the half life for uranium is 6 into 10 power 9s. On the other hand half life for polonium is 0.5 micro second. Note that although the energy of the emitted alpha particle varies only by a factor of 2 lifetime varies by several orders of magnitude.

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Transmission probability (WKB)

WKB: $\gamma = \frac{1}{\hbar} \int_{r_1}^{r_2} \sqrt{2m[V(r) - E]} dr$

- $r_1 =$ radius of parent nucleus X
- At point r_2 : $\frac{1}{4\pi\epsilon_0} \frac{(Ze)(2e)}{r_2} = E$
- $\gamma = \frac{\sqrt{2mE}}{\hbar} \int_{r_1}^{r_2} \sqrt{\frac{r_2}{r} - 1} dr$
- Assuming $r_1 \ll r_2$: $\gamma \approx \frac{\sqrt{2mE}}{\hbar} \left[\frac{\pi}{2} r_2 - 2\sqrt{r_1 r_2} \right] = K_1 \frac{Z}{\sqrt{E}} - K_2 \sqrt{Z r_1}$
- Let v be velocity: time between two collisions with wall $\frac{2r_1}{v}$
- Collision frequency: $\frac{v}{2r_1}$, probability of alpha emission/time: $\frac{v}{2r_1} e^{-2\gamma}$
- Lifetime of parent nucleus: $\tau_{1/2} = \frac{2r_1}{v} e^{2\gamma} \Rightarrow \log \tau_{1/2} = \frac{4r_1}{v} \gamma$
- $\log \tau_{1/2} = \left(\frac{4r_1 K_1 Z}{v} \right) \frac{1}{\sqrt{E}} - \frac{4r_1 K_2 \sqrt{Z r_1}}{v}$
- Gamow's theory of alpha decay indeed captures Geiger-Nuttall law

Remember that alpha particle is emitted from the current nucleus x which is converted to some other nucleus y. Let us try to estimate the lifetime of parent nucleus using Gamow's theory let Z times e be the charge of remaining nucleus y after the alpha particle escapes the parent nucleus. Charge of the alpha particle is 2e thus once the particle travels from r 1 to r 2 it is free from the nuclear binding.

And Coulomb repulsion by the remaining nuclear charge pushes the particle further away the coulomb repulsion is given by $\frac{1}{4\pi\epsilon_0} \frac{Ze \cdot 2e}{r}$ where Z is the charge of the remaining nucleus and 2e, 2e is the charge of the alpha particle divided by r. Applying WKB approximation we can find the transmission probability p which is equal to $e^{-2\gamma}$ where gamma is calculated from this integral.

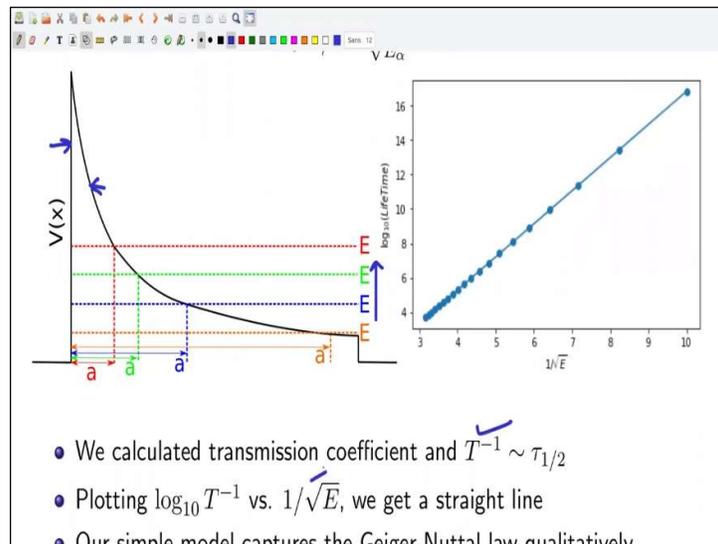
In the integral the lower limit r 1 is the radius of the parent nucleus x which is of the order of 10 fermi where 1 for fermi is 10 power -15 meter. The point at which the particle finally escapes the energy of the particle should be equal to the potential energy that is at this point the potential energy is equal to the energy of the particle. Thus r 2 the upper limit of this integral can be obtained by equating E with the coulomb repulsion.

Then gamma can be written as this integral square root of 2 me by h bar integral r 1 to r 2 square root of $\frac{r_2}{r} - 1$ dr generally r 1 is much smaller than r 2 and in that case gamma can be approximately written as $K_1 \frac{Z}{\sqrt{E}} - K_2 \sqrt{Z r_1}$ where K 1 and K 2 are constants. If V is the velocity of the alpha particle time between two collisions with the wall is given by $\frac{2r_1}{V}$ where r 1 is the radius of the nucleus.

Inverse of this quantity is the collision frequency which is equal to V by $2 r 1$. Probability of alpha emission per unit time is a product of collision frequency and transmission probability given by V divided by $2 r 1$ times e power $- 2 \gamma$ where e power $- 2 \gamma$ is the transmission probability. Lifetime of the parent nucleus is inversely proportional to the probability of the alpha emission. Thus we can write half life $\tau_{1/2}$ is equals to $2 r 1$ divided by V times e power 2γ .

Taking log on both the sides we get log of tau is equals to $4 r 1$ divided by V times γ . Now replacing the value of γ from this equation we can write log of tau is equals to $4 r 1 K 1 Z$ divided by V times 1 by square root of e - some term which is not a function of energy. Thus Gamow's theory of alpha decay indeed captures the Geiger-Nuttall law.

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Let us see whether our code can qualitatively capture Geiger-Nuttall law. Our potential profile looks very similar to what is used in Gamow's theory. The vertical line shows the finite potential wall then we have a potential which is become continuously in space. This is qualitatively similar to Coulomb repulsion. We increase the energy of the alpha particle from low to high and calculate the transmission coefficient.

The transmission coefficient is inversely proportional to the lifetime term. Now according to Geiger-Nuttall law if we plot log of tau as a function of 1 by square root of e alpha where e alpha is the energy of the alpha particle then we should get a straight line. Let us plot log of p

inverse as a function of $1/\sqrt{E}$. If we get a straight line that will indicate that our model is good enough to capture the Geiger-Nuttall law.

Let us run the code and plot $\log t$ inverse as a function of $1/\sqrt{E}$. Thus plotting $\log t$ inverse versus $1/\sqrt{E}$ we get a nice straight line as shown here. Thus our simple model captures the Geiger-Nuttall law qualitatively.