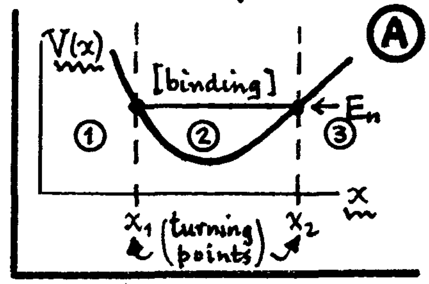
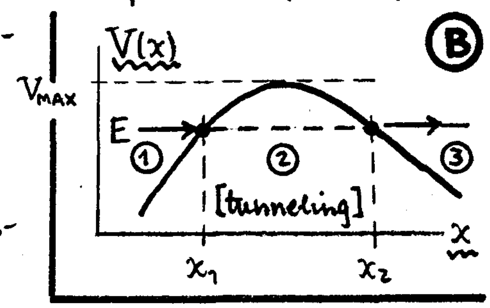
Applications of the WKB Approximation: QM Tunneling. [ref. Davydov, ¶24.]

1) We have seen how the WKB method yields a general quantization rule for the (approximate) calculation of the bound state energies of a particle of mass m in any attractive potential well $V(x)$, via the Bohr-Sommerfeld formula...



$$\boxed{\int_{x_1}^{x_2} \sqrt{2m[E_n - V(x)]}\, dx = (n+\tfrac{1}{2})\pi\hbar}\ ; \quad n = 0,1,2,\ldots \quad (1)$$

(x_1 & x_2 are the turning pts, ∀ $V(x_1) = E_n = V(x_2)$). Another general problem of this type is the inverse of the well problem, namely the case of a repulsive potential barrier. Here, a free particle of energy $E < V_{MAX}$ encounters a barrier $V(x)$ as shown. The question of interest here is: if the particle is incident from the left in region ① @ $E < V_{MAX}$, will it ever be found in region ③ -- i.e. will it "penetrate" the barrier? Classically, this cannot happen; QMly, it can. We shall now use the WKB method to calculate the transmission coefficient for the particle penetrating (i.e. tunneling through) the potential barrier.



REMARKS

1. A criterion for accuracy of the WKB method for both problems Ⓐ & Ⓑ above may be stated as follows: the distance $(x_2 - x_1)$ between the turning points must be big enough to contain a "large" number of DeBroglie wavelengths $\lambda = 2\pi/|k|$ for the particle. This statement concerns the width of the regions ② in the above sketches. The WKB method will tend to become inaccurate in problem Ⓐ as the particle approaches the bottom of the well ($n \to 0$); the WKB method will become less accurate in problem Ⓑ as the particle approaches the top of the barrier ($E \to V_{MAX}$).

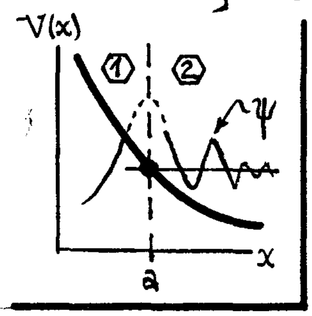
This accuracy criterion was discussed on p. W12.

(next page)

WKB: Remarks on Barrier Problem.

2. The barrier & well problems differ in one important respect. In the well problem Ⓐ, we dealt only with the WKB decaying exponentials $\exp[-\int K(x')dx']$ in the exterior regions ①&③; these fcns had to vanish far to the left of x_1 and far to the right of x_2. In the barrier problem Ⓑ, the WKB exponential solution region is ②, and since this region is finite, both decaying & growing solutions $\exp[\mp\int K(x')dx']$ are admissible in region Ⓑ-②. Thus, for the barrier problem, we will use all the connection formulas in Eqs.(27A) & (27B) on p. W 11 to connect regions ① ↔ ② and ② ↔ ③.†

It is worth noting that the WKB Connection Formulas are not just simple analytic continuations of ψ from the nonclassical to classical regions. E.g.

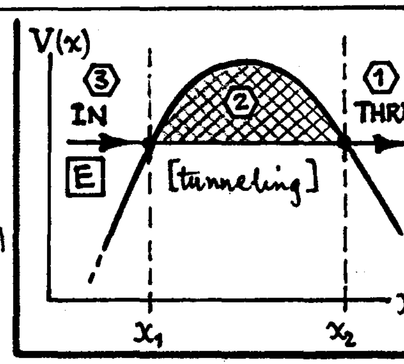


$$\left.\begin{array}{l}\text{analytic}\\ \text{continuation}\end{array}\right\}\; e^{-\int_x^a K(x')dx'} \rightarrow e^{+i\phi(x)},\quad \phi(x)=\int_a^x k(x')dx' \;\int \psi \text{ moving to right only;}$$

$$\left.\begin{array}{l}\text{WKB}\\ \text{connection}\end{array}\right\}\; e^{-\int_x^a K(x')dx'} \rightarrow 2\sin\left(\phi+\frac{\pi}{4}\right)=\underbrace{\left(e^{-\frac{i\pi}{4}}\right)e^{i\phi}+\left(e^{\frac{i\pi}{4}}\right)e^{-i\phi}} \qquad (2)$$

The WKB result is a standing wave, with both R-ward & L-ward components.

2) We now proceed to calculate the transmission coefficient for the barrier problem sketched at right. We imagine a particle incident from the left at energy E in region ③, partially reflected and partially transmitted at point x_1, tunneling thru region ②, and ultimately penetrating to x_2 to emerge in region ① travelling to the right. The wavenumbers in the various regions are:



$$\rightarrow k(x)=\sqrt{(2m/\hbar^2)[E-V(x)]},\ \text{in ③&①};\quad K(x)=\sqrt{(2m/\hbar^2)[V(x)-E]},\ \text{in ②}. \qquad (3)$$

† To make this connection for the well problem, we only need the first of each of Eqs.(27A)&(27B), viz. $e^{-(\;)} \leftrightarrow \sin(\;)$. Now we also need $e^{+(\;)} \leftrightarrow \cos(\;)$ forms.

WKB: Details of Barrier Penetration (per WKB).

Region ① is the simplest: m travels only to the right, so we write a particular WKB solution in the form... with A = arbitrary const...

$$\psi_1(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\left[\int_{x_2}^{x} k(x')dx' + \frac{\pi}{4}\right]} \leftarrow \text{righthand traveling wave in region ①.}$$

or//

$$\psi_1(x) = \frac{A}{\sqrt{k}}\left\{\cos\left[\int_{x_2}^{x} k\,dx' + \frac{\pi}{4}\right] + i\sin\left[\int_{x_2}^{x} k\,dx' + \frac{\pi}{4}\right]\right\}, \text{ in ①.} \tag{4}$$

The phase factor $\pi/4$ is introduced to facilitate application of the connection formulas (since A is in general complex, we are free to extract this phase factor from it).

Now the connection formulas [Eqs. (27A) & (27B) on p. W 11] imply that when we go from region ① to region ②, in Eq. (4) the $\cos \rightarrow e^{+}$ and $\sin \rightarrow \frac{1}{2}e^{-}$, with $k(x)$ replaced by $K(x)$. Thus, the WKB solution in region ② is:

$$\rightarrow \psi_2(x) = \frac{A}{\sqrt{K}}\left\{e^{+\int_x^{x_2} K(x')dx'} + \frac{i}{2}\, e^{-\int_x^{x_2} K(x')dx'}\right\}. \tag{5}$$

To continue this ψ into the incident region ③, we will need integrals $\int_{x_1}^{x}$ referred to the lefthand turning point. We note that...

$$\int_x^{x_2} = \int_{x_1}^{x_2} - \int_{x_1}^{x}. \quad \text{Define: } \boxed{Q = \exp\left[-\int_{x_1}^{x_2} K(x')dx'\right]}.$$

$$\text{So//} \rightarrow \psi_2(x) = \frac{A}{\sqrt{K}}\left\{\frac{1}{Q}\left(e^{-\int_{x_1}^{x} K(x')dx'}\right) + \frac{i}{2}Q\left(e^{+\int_{x_1}^{x} K(x')dx'}\right)\right\}, \text{ in ②.} \tag{6}$$

To join ψ_2 in Eq. (6) to ψ_3 in region ③, the connection formulas prescribe for the exponentials: $e^{(-)} \rightarrow 2\sin$, $e^{(+)} \rightarrow \cos$. Then we have, for $x < x_1$...

$$\psi_3(x) = \frac{A}{\sqrt{k(x)}}\left\{\frac{2}{Q}\sin\left[\int_x^{x_1} k(x')dx' + \frac{\pi}{4}\right] + \frac{i}{2}Q\cos\left[\int_x^{x_1} k(x')dx' + \frac{\pi}{4}\right]\right\}$$

or//

$$\psi_3(x) = \frac{A}{\sqrt{k}}\left\{\underbrace{\left(\frac{1}{Q} + \frac{Q}{4}\right)e^{+i\left[\int_{x_1}^{x} k\,dx' + \frac{\pi}{4}\right]}}_{\text{incident wave (travels to RIGHT)}} + \underbrace{\left(\frac{1}{Q} - \frac{Q}{4}\right)e^{-i\left[\int_{x_1}^{x} k\,dx' + \frac{\pi}{4}\right]}}_{\text{reflected wave (travels to LEFT)}}\right\}. \tag{7}$$

WKB: Barrier Transmission Coefficient T.

NOTE: Traveling "right" & "left" in Eq. (7) is heralded by the $e^{\pm ikx}$ factor. This convention relates to the fact that planewaves $e^{\pm ikx - \omega t}$ travel right & left, resp.

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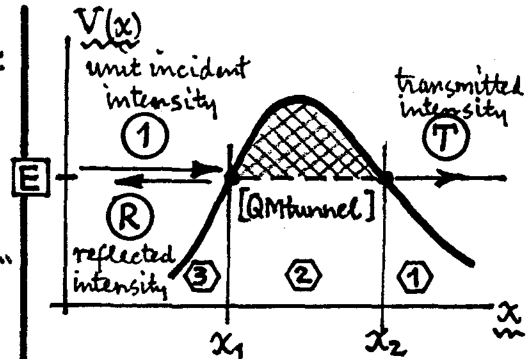
3) Now compare the rightward traveling parts of the incident wave ψ_3 in Eq. (7) and the transmitted wave ψ_1 in Eq. (4). The intensity ratio is...

$$\rightarrow T = |\psi_1(\text{right})|^2 \div |\psi_3(\text{right})|^2 = 1\Big/\left(\frac{1}{Q}+\frac{Q}{4}\right)^2 = Q^2\Big/\left(1+\frac{Q^2}{4}\right)^2 \quad \text{Q defined in Eq. (6).} \tag{8}$$

T is called the transmission coefficient for the barrier: it is the transmitted intensity per unit incident intensity for the particle (mass m, energy E), and it gives the probability that the incident particle will "tunnel" through the barrier (region ②) and appear on the other side.



QM tunneling factor is:

$$Q = \exp\left[-\int_{x_1}^{x_2} K(x)\,dx\right],$$

w/ $K(x) = \sqrt{(2m/\hbar^2)[V(x)-E]}$.

Then: $T \simeq Q^2$, $R \simeq 1 - Q^2$.

We can also define a reflection coefficient R as the ratio $|\psi_3(\text{left})|^2 \div |\psi_3(\text{right})|^2$. From Eq. (7)...

$$\rightarrow R = \left(\frac{1}{Q}-\frac{Q}{4}\right)^2 \div \left(\frac{1}{Q}+\frac{Q}{4}\right)^2 = \left(1-\frac{Q^2}{4}\right)^2\Big/\left(1+\frac{Q^2}{4}\right)^2. \tag{9}$$

We note that $T + R = 1$ (Eq. (8) + Eq. (9) = 1, conservation of probability).

Also note that Q is very small if our WKB calculation is to work. That's because the barrier width $(x_2 - x_1) \gg \lambda$, as remarked on p. W12. Thus...

$$\rightarrow \int_{x_1}^{x_2} K(x)\,dx = 2\pi \int_{x_1}^{x_2} dx/|\lambda(x)| = 2\pi \frac{(x_2 - x_1)}{|\lambda|_{AV}} \gg 1 \Rightarrow \underline{\underline{Q = e^{-\int_{x_1}^{x_2} K\,dx} \ll 1}}. \tag{10}$$

Here $|\lambda|_{AV}$ is the mean de Broglie $|\lambda|$ inside the barrier. By the nature of the WKB approxn, the calc$^{\underline{n}}$ is good only if $\int K\,dx \to$ large. Anyway, $Q \ll 1$ means:

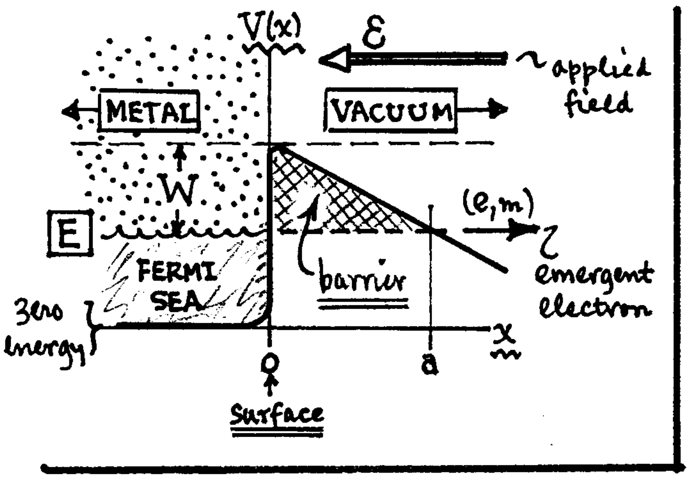
$$\boxed{T \simeq Q^2 = \exp\left\{-\frac{2}{\hbar}\int_{x_1}^{x_2} \sqrt{2m[V(x)-E]}\,dx\right\}} \quad \text{WKB barrier transmission coefficient,} \tag{11}$$

from Eq. (8). Notice that when $\hbar \to 0$ (classical limit), $T \to 0$, as it should.

WKB: Field Emission from a Metal Surface.

ref. Davydov, pp. 85-86

4) As an example of the use of Eq. (11) for T, we look at "field emission", where electrons are pulled out of a metal surface by application of a strong external electric field $\mathcal{E}$. The appropriate energy diagram is...



E = highest energy of an electron in Fermi sea.

W = "work function" of metal ($W = e\varphi$). This is the height of the barrier.

When the external field $\mathcal{E}$ is applied, the total external (vacuum) potential may be written:

$$V(x) = E + W - e\mathcal{E}x, \text{ for } x > 0. \tag{12}$$

Near the metal's surface ($x=0$), $V(x)$ is modified by surface irregularities (N.B. "irregularity" is a synonym for surface science). We assume this region is small compared to the total barrier width a, which is found from...

$$\rightarrow @ \; x = a : \; V(x) - E = W - e\mathcal{E}x = 0 \Rightarrow \underline{\underline{a = W/e\mathcal{E}}}. \tag{13}$$

Most of the emitted e's in fact come from the top of the Fermi sea, and the emission current density J will be proportional to the probability that the e's tunnel through the indicated barrier. According to Eq. (11)...

$$J \propto T \simeq \exp\left\{-\frac{2}{\hbar}\int_0^a \sqrt{2m[V(x)-E]}\,dx\right\} = \exp\left\{-\frac{2}{\hbar}\sqrt{2m}\int_0^{W/e\mathcal{E}} \sqrt{W - e\mathcal{E}x}\,dx\right\}$$

by

$$\boxed{J \propto \exp\left\{-\frac{4}{3}\left(\frac{\sqrt{2me}}{\hbar}\right)\varphi^{3/2}/\mathcal{E}\right\}}, \quad \varphi = W/e \text{ [work fcn in volts]} \tag{14}$$

So, for field emission, the prediction is: $\log J = -(\text{const})\cdot \varphi^{3/2}/\mathcal{E}$, as sketched at right. This result agrees semi-quantitatively with exptal data [see, e.g., p. 24 of Kaminsky "Atomic & Ionic Impact Phenomena on Metal Surfaces" (Academic Press, 1965)].