

E6510: Finding energy levels using WKB

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The problem:

Find, using the WKB approximation, the energy levels of a one dimensional problem with a potential of $V(x) = \text{sign}(\alpha) \cdot x^\alpha$, $x \geq 0$.

For what values of α is there a floor?

In particular, discuss the cases of $\alpha = 2, 0, -1$

The solution:

According to the WKB approximation: $\int_{x_1}^{x_2} P(x) dx = \pi \hbar \left(n + \frac{1}{2}\right)$. For x_1, x_2 - the turning points in the energy E_n .

$$P(x) = \sqrt{2m[E_n - V(x)]} = \sqrt{2m[E_n - \text{sign}(\alpha) \cdot x^\alpha]}$$

We will notice that for $\alpha > 0$, $E_n > 0$. And for $\alpha < 0$, $E_n < 0$ (In this case $E_n > 0$ is allowed, but these are not bound states).

$$x_1 = 0 \quad x_2 = (\text{sign}(\alpha) \cdot E_n)^{1/\alpha}$$

We will refer to $\text{sign}(\alpha)$ as S from now on.

$$\begin{aligned} \int_{x_1}^{x_2} P(x) dx &= \sqrt{2m} \int_0^{(SE_n)^{1/\alpha}} \sqrt{E_n - S \cdot x^\alpha} dx = \sqrt{2m} (SE_n)^{\frac{1}{2}} \int_0^{(SE_n)^{1/\alpha}} \sqrt{S - \frac{x^\alpha}{E_n}} dx = \\ &= \sqrt{2m} (SE_n)^{\frac{1}{2}} \int_0^{(SE_n)^{1/\alpha}} \sqrt{S - S \left(\frac{x}{(SE_n)^{1/\alpha}} \right)^\alpha} dx = \\ &= \sqrt{2m} (SE_n)^{\frac{1}{2} + \frac{1}{\alpha}} \int_0^1 \sqrt{S(1 - t^\alpha)} dt \end{aligned}$$

We will define the integral: $C(\alpha) = \int_0^1 \sqrt{S(1 - t^\alpha)} dt$ and we shall get:

$$\int_{x_1}^{x_2} P(x) dx = \sqrt{2m} (SE_n)^{\frac{1}{2} + \frac{1}{\alpha}} C(\alpha) = \pi \hbar \left(n + \frac{1}{2}\right)$$

Extracting E_n from the expression we get a solution for all $\alpha \neq 0$:

$$E_n = S \left(\frac{\pi \hbar \left(n + \frac{1}{2}\right)}{\sqrt{2m} C(\alpha)} \right)^{\frac{2\alpha}{\alpha+2}}$$

The condition for floor to exist is the convergence of the integral defining $C(\alpha)$.

The reason is when the integral converges, it means that until certain energy, there is a finite area in the phase domain, and therefore a finite number of allowed states, hence, there has to be a ground

state (floor). When the integral does not converge, there is infinite area in the phase domain, which means infinite number of states, hence, no ground state.

$$\text{Integrand}\{C(\alpha)\} = \sqrt{S(1-t^\alpha)} \approx \begin{cases} t^{\frac{\alpha}{2}} & \alpha < 0 \\ 1 & \alpha > 0 \end{cases} \text{ When } t \rightarrow 0.$$

Therefore, the integral always converges for $\alpha > 0$, but for $\alpha < 0$ the integral only converges for $\alpha > -2$.

Conclusion: There is a floor for each $\alpha > -2$.

$\alpha = 2$, Harmonic Oscillator

$$C(2) = \frac{\pi}{4}$$

$$E_n = 2\sqrt{\frac{2}{m}}\hbar\left(n + \frac{1}{2}\right) = 2\hbar\omega\left(n + \frac{1}{2}\right)$$

$$\left\{1 = \frac{1}{2}m\omega^2 \Rightarrow \omega = \sqrt{\frac{2}{m}}\right\}$$

We got the expected result with an additional factor of 2, coming from the fact we only regarded the positive half of the x axis.

$\alpha = -1$, Hydrogen Atom

$$C(-1) = \frac{\pi}{2}$$

$$E_n = -\left(\frac{\sqrt{2}\hbar\left(n+\frac{1}{2}\right)}{\sqrt{m}}\right)^{-2} = -\frac{m}{2\hbar^2\left(n+\frac{1}{2}\right)^2}$$

We got the spectrum of the hydrogen atom, except the $\frac{1}{2}$ which was added to the denominator.

For the case of $\alpha = 0$ we will solve separately.

$$V(x) = 0 \quad P(x) = \sqrt{2mE_n}$$

$$\int_0^L P(x) dx = \int_0^L \sqrt{2mE_n} dx = L\sqrt{2mE_n} = \pi\hbar\left(n + \frac{1}{2}\right) \Rightarrow E_n = \frac{\pi^2\hbar^2\left(n+\frac{1}{2}\right)^2}{2mL^2}$$

We got the spectrum of an infinite potential well with soft boundary conditions.

$$\Delta E_n = E_n - E_{n-1} = \frac{\pi^2\hbar^2}{2mL^2} \left[\left(n + \frac{1}{2}\right)^2 - \left(n - \frac{1}{2}\right)^2 \right] = \frac{\pi^2\hbar^2 n}{mL^2}$$

$$\lim_{L \rightarrow \infty} \Delta E_n = 0$$

Meaning that in the limit of $L \rightarrow \infty$ the gap between neighboring energy levels is reduced to zero, and we get a continuous spectrum.

Of course there is a floor since the energy has to be positive which fits the 'floor condition' from the general case.