Ex6511: Finding energy eigenstates in a semi-classical approximation

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The problem:

A particle of mass M is free to move in 1 Dimension. Using the WKB approximation find the energy eigenstates E_n of the particle in the following cases:

(1) The potential is $V(x) = c|x|^\alpha$ where $\alpha > 0$. use the following notation: $B(\alpha) = \int_0^1 \sqrt{1-x^\alpha}dx$.
(2) A potential well in the interval $[-a, a]$ with a potential floor of $V(x) = V_0 sign(x)$. It is enough to write the answer for energy levels above V_0.
(3) Bonus question: in section (2) calculate the eigenenergies using perturbation theory up to second order.

The solution:

(1) In the WKB approximation bounded states satisfy the condition:

$$\int_{x_1}^{x_2} p(x)dx = \pi(n+\frac{1}{2})$$

The turning points are:

$$x_1 = -(\frac{E}{c})^{\frac{1}{\alpha}}$$

$$x_2 = (\frac{E}{c})^{\frac{1}{\alpha}}$$

And the momentum:

$$p(x) = \sqrt{2M(E-V(x))} = \sqrt{2M(E-c|x|^\alpha)}$$

Calculating the integral:

$$\int_{-(\frac{E}{c})^{\frac{1}{\alpha}}}^{(\frac{E}{c})^{\frac{1}{\alpha}}} \sqrt{2M(E-c|x|^\alpha)}dx = \sqrt{2ME}\Big[\int_{-(\frac{E}{c})^{\frac{1}{\alpha}}}^{0} \sqrt{(1-\frac{c}{E}(-x)^\alpha)}dx + \int_0^{(\frac{E}{c})^{\frac{1}{\alpha}}} \sqrt{1-\frac{c}{E}x^\alpha dx}\Big]$$

$$= 2B(\alpha)(\frac{E}{c})^{\frac{1}{\alpha}}\sqrt{2ME}$$

So we get:

$$2B(\alpha)(\frac{E}{c})^{\frac{1}{\alpha}}\sqrt{2ME} = \pi(n+\frac{1}{2})$$

Solving for E_n:

$$E_n = \left[\frac{\pi(n+\frac{1}{2})}{\sqrt{8M}B(\alpha)}c^{\frac{1}{\alpha}}\right]^{\frac{2\alpha}{\alpha+2}}$$

(2) In the case of a potential well the walls are "hard" therefore the equation for the bound energies is:

$$\int_{x_1}^{x_2} p(x)dx = \pi n$$

$$\int_{-a}^{a}\sqrt{2M(E-V(x))}dx = \int_{-a}^{0}\sqrt{2M(E+V_0)}dx + \int_{0}^{a}\sqrt{2M(E-V_0)}dx$$

$$a\sqrt{2M(E+V_0)} + a\sqrt{(2M(E-V_0)} = \pi n$$

Solving the equation for E gives:

$$E_n = \epsilon_n + \frac{V_0^2}{4\epsilon_n}$$

where $\epsilon_n = \frac{\pi^2 n^2}{8Ma^2}$

(3) We look at a symmetrical potential well with a perturbation of $V(x) = V_0 sign(x)$.
The eigenstates of the unperturbated Hamiltonian:
odd n: $\Psi_n = \frac{1}{\sqrt{a}}\cos k_n x$
even n: $\Psi_n = \frac{1}{\sqrt{a}}\sin k_n x$
where: $k_n = \frac{\pi n}{2a}$ and the energy is $\epsilon_n = \frac{\pi^2 n^2}{8Ma^2}$
Finding the matrix elements of the perturbation:
On the diagonal:

$$V_{nn} = \langle n|v|n\rangle = \frac{1}{a}\int_{-a}^{a}\cos^2(k_n x)V(x)dx = \frac{1}{a}\int_{-a}^{a}\sin^2(k_n x)V(x)dx = 0$$

because $\cos^2(k_n x)V(x)$ and $\sin^2(k_n x)V(x)$ are odd functions.
Therfore:

$$E_n^{[1]} = V_{nn} = 0$$

Off diagonal elements:

$$m = odd, n = odd : \frac{1}{a}\int_{-a}^{a}\cos(k_m x)\cos(k_n x)V(x)dx = 0$$

$$m = even, n = even : \frac{1}{a}\int_{-a}^{a}\sin(k_m x)\sin(k_n x)V(x)dx = 0$$

Because the integrands in both integrals are odd functions.

$$m = odd, n = even : \frac{1}{a}\int_{-a}^{a}\cos(k_m x)\sin(k_n x)V(x)dx =$$

$$= \frac{V_0}{2a}\left[-\int_{-a}^{0}\sin((k_n+k_m)x) + \sin((k_n-k_m)x)dx + \int_{0}^{a}\sin((k_n+k_m)x) + \sin((k_n-k_m)x)dx\right]$$

$$= \frac{-V_0}{a}\left[\frac{\cos((k_n+k_m)x)}{k_n+k_m} + \frac{\cos((k_n-k_m)x)}{k_n-k_m}\right]_0^a$$

We notice that for $x = a$ the expression equals 0 because $(k_n \pm k_m)a = \frac{2l+1}{2}\pi$ for an integer l.
So we are left with:

$$V_{mn} = \frac{2V_0}{\pi}\Big(\frac{1}{n+m} + \frac{1}{n-m}\Big) = \frac{4V_0}{\pi}\Big(\frac{n}{n^2-m^2}\Big)$$

For $m = even, n = odd$, we get the same result but with a replacement of m with n:

$$V_{mn} = \frac{2V_0}{\pi}\Big(\frac{1}{n+m} + \frac{1}{m-n}\Big) = \frac{4V_0}{\pi}\Big(\frac{m}{m^2-n^2}\Big)$$

The second order correction of the energy:

$$E_n^{[2]} = \sum_{m(\neq n)} \frac{|V_{mn}|^2}{\epsilon_n - \epsilon_m}$$

For the symmetrical states (odd n) we get:

$$E_n^{[2]} = \sum_{m(\neq n)} \Big(\frac{4V_0 m}{\pi(m^2-n^2)}\Big)^2 \frac{8Ma^2}{\pi^2(n^2-m^2)} = \frac{V_0^2}{\epsilon_n}\frac{16}{\pi^2}\sum_{l=1}^{\infty}\frac{n^2(2l)^2}{(n^2-(2l)^2)^3} = \frac{V_0^2}{\epsilon_n}C_s(n)$$

For the antisymmetrical states (even n) we get:

$$E_n^{[2]} = \sum_{m(\neq n)} \Big(\frac{4V_0 n}{\pi(n^2-m^2)}\Big)^2 \frac{8Ma^2}{\pi^2(n^2-m^2)} = \frac{V_0^2}{\epsilon_n}\frac{16}{\pi^2}\sum_{l=0}^{\infty}\frac{n^4}{(n^2-(2l+1)^2)^3} = \frac{V_0^2}{\epsilon_n}C_{as}(n)$$

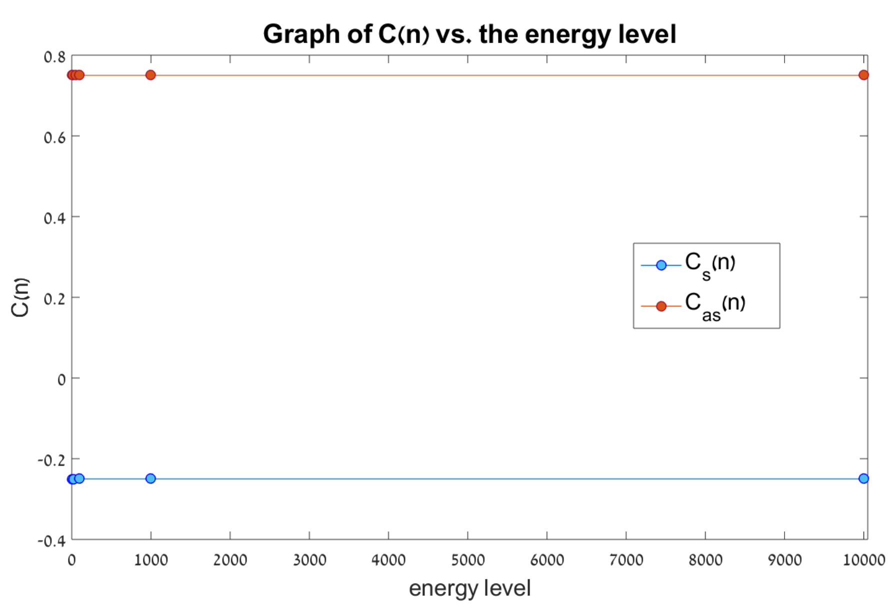
It is clear that the most significant contribution to the sum is when $m = n \pm 1$. Therfore, we calculate the contribution of these elements for $C_s(n)$ and $C_{as}(n)$ in the limit $n \to \infty$:
For $C_s(n)$:

$$\lim_{n\to\infty}\frac{16}{\pi^2}\Big(\frac{n^2(n+1)^2}{(n^2-(n+1)^2)^3} + \frac{n^2(n-1)^2}{(n^2-(n-1)^2)^3}\Big) \cong -0.203$$

For $C_{as}(n)$:

$$\lim_{n\to\infty}\frac{16}{\pi^2}\Big(\frac{n^4}{(n^2-(n+1)^2)^3} + \frac{n^4}{(n^2-(n-1)^2)^3}\Big) \cong 0.608$$

In order to improve the accuracy, we approximate the sums using Matlab for different energy levels. The results are shown in the following graph:



We get $C_s(n) = -\frac{1}{4}$ and $C_{as}(n) = \frac{3}{4}$ for all values of n.
The energy up to second order perturbation is:
for the symmetrical states:

$$E_n = \epsilon_n - \frac{V_0^2}{4\epsilon_n}$$

for the antisymmetrical states:

$$E_n = \epsilon_n + \frac{3V_0^2}{4\epsilon_n}$$

Comparing the WKB approximation to perturbation theory, we see that it is the algebraic average of the symmetric and antisymmetric states.