One problem in the final of Phy. 731.

A particle with mass m is moving in the potential $U(x) = m\omega^2 x^2(1 - x/a)/2$ from a quasi-stationary state near $x = 0$ in the limit $a \gg \sqrt{\hbar/m\omega}$. To determine the escape rate, one first compute the transmission probability $T(E)$ for a particle with energy $E > 0$ moving from left in potential $U(x)\theta(x)$ where $\theta(x)$ is the Heaviside function. The escape rate can be estimated by the product of $T(E_n)$ and the attempt rate $\omega/2\pi$ where $E_n = \hbar\omega(n + 1/2)$. Evaluate Γ_1/Γ_0.

By WKB matching, the transmission probability is given by

$$T(E) = \exp(-\frac{2}{\hbar}\int_{x_1(E)}^{x_2(E)} \sqrt{2m(U(x) - E)}dx)$$

where x_1, x_2 are the zeros of the thing in the square root. Then, the result is $T(E_1)/T(E_0)$.

Here, I would like to deviate to talk about several integral types that may arise in WKB.

1 First type integral

Compute the integral

$$I = \int_{y_1}^{y_2} \sqrt{1 - y^2 - \varepsilon dy}$$

to $O(\varepsilon)$.

Usually, one may do the expansion

$$I = \int_{y_1}^{y_2} \sqrt{1 - y^2}(1 - \frac{\varepsilon}{2(1 - y^2)})dy + O(\varepsilon^2)$$

and substitute $y_1 \to y_1(0), y_2 \to y_2(0)$.

One may want to justify this. Actually, if one takes the derivative $I'(0) = \int_{y_1(0)}^{y_2(0)}(\cdots)'|_{\varepsilon=0}dy$. The boundary terms vanish since they are the zeros of the integrand.

The expansion therefore is

$$I = I(0) + I'(0)\varepsilon + O(\varepsilon^2) = \int_{-1}^{1}(\sqrt{1 - y^2} - \frac{\varepsilon}{2\sqrt{1 - y^2}})dy + O(\varepsilon^2)$$
$$= \frac{\pi}{2} - \frac{\pi\varepsilon}{2} + O(\varepsilon^2)$$

This method actually works in many situations.

2 Second type

Let's consider this integral

$$I(a) = \int_{y_1}^{y_2} \sqrt{a - y^2 - \varepsilon y^4} dy$$

Compute $\Delta I/\Delta a$ to $O(\varepsilon)$.

One may want to try two methods. The first is to expand around ε first and get

$$\begin{aligned} I &= \int_{y_1(\varepsilon=0)}^{y_2(\varepsilon=0)} \sqrt{a - y^2}(1 - \frac{\varepsilon y^4}{2(a - y^2)}) dy + O(\varepsilon^2) \\ &= \frac{\pi}{2} a - \frac{3\pi a^2 \varepsilon}{16} + O(\varepsilon^2) \end{aligned}$$

Then, one can take derivative on a happily.

However, somebody(like me) might try to get the expression as far as possible and might tempted to compute the accurate expression first. Naively, one take derivative of I on a first and then throw away the boundary terms since y_1, y_2 are zeros of the integrand and have

$$I'(a) = \int_{y_1}^{y_2} \frac{1}{2\sqrt{a - y^2 - \varepsilon y^4}} dy$$

Now, expand this expression about ε. However, one sees that the $O(\varepsilon)$ term has expression as

$$\int_{y_1}^{y_2} \frac{y^4}{(a - y^2)^{3/2}} dy$$

Unfortunately, this integral diverges. This happens because $y_2 = \sqrt{a} + \delta\varepsilon + O(\varepsilon^2)$. Plugging in, one can get δ. This root is differentiable with respect to a and probably, throwing away is fine(?). Well what is the issue?

Another method is to scale first. Let $y = \sqrt{a} z$ and one has

$$I(a; \varepsilon) = \int_{z_1}^{z_2} a\sqrt{1 - z^2 - a\varepsilon z^4} dz$$

Taking derivative on a in this expression, one can have the correct exact expression of $I'(a)$ now. Take derivative and also throw away the boundary terms since the limits are the roots of the integrand, we have

$$\frac{\Delta I}{\Delta a} = \int_{z_1}^{z_2} \sqrt{1 - z^2 - a\varepsilon z^4} dz + a \int_{z_1}^{z_2} \frac{-\varepsilon z^4}{2\sqrt{1 - z^2 - a\varepsilon z^4}} dz$$

Expand around $\varepsilon = 0$, one has

$$\left(\int_{-1}^{1} \sqrt{1-z^2}dz - \int_{-1}^{1} \frac{a\varepsilon z^4}{2\sqrt{1-z^2}}dz\right) - a\varepsilon \int_{-1}^{1} \frac{z^4}{2\sqrt{1-z^2}}dz$$
$$= \frac{\pi}{2} - a\varepsilon \int_{-1}^{1} \frac{z^4}{\sqrt{1-z^2}}dz = \frac{\pi}{2} - a\varepsilon\frac{3\pi}{8}$$

This agrees with the first integral. Now, let's go back to check the issue. Let

$$J(\varepsilon) = \int_{y_1}^{y_2} \frac{1}{2\sqrt{a-y^2-\varepsilon y^4}}dy$$

we see that we can't have $J'(0)$ by taking derivative directly because the integrand is infinity at the limits. That means we can't expand the integrand only with the boundary terms thrown away. If we do change of variables, we have

$$J(\varepsilon) = \int_{z_1}^{z_2} \frac{1}{2\sqrt{1-z^2-\varepsilon a z^4}}dz$$

Is this the same as the derivative above? For $\varepsilon = 0$, yes; but for $\varepsilon \neq 0$, unknown. This needs to be checked in the future.

3 Third type

Consider the integral

$$I(\varepsilon) = \int_{y_1}^{y_2} \sqrt{y^2(1-y)-\varepsilon}dy$$

Again, if one expand the integrand and set $y_1 = 0, y_2 = 1$, one has

$$I(\varepsilon) = \int_{0}^{1} \sqrt{y^2(1-y)}(1 - \frac{\varepsilon}{2(y^2(1-y))})dy + O(\varepsilon^2)$$

but the second integral diverges around $y = 0$.

Investigating the integral, one notices that $y_1 = \sqrt{\varepsilon} + o(\sqrt{\varepsilon})$. That means the boundary terms can not be thrown away when one take $I'(\varepsilon)$.

If one notices this, one can see that the leading term is just

$$\int_{\sqrt{\varepsilon}}^{1} y\sqrt{1-y}dy = 2\left(\frac{1}{3}(1-\sqrt{\varepsilon})^{3/2} - \frac{1}{5}(1-\sqrt{\varepsilon})^{5/2}\right)$$

Unfortunately, this integral is just $I(\varepsilon = 0) + O(\varepsilon)$, there is no $\sqrt{\varepsilon}$ term. The main contribution actually comes from the next term which is $O(\varepsilon \ln(\varepsilon))$ lager than $O(\varepsilon)$ term here.

One can compute that

$$-\int_{\sqrt{\varepsilon}}^{1} \frac{\varepsilon}{2y\sqrt{1-y}} dy = -\frac{\varepsilon}{2} \ln\left(\frac{1+\sqrt{1-\sqrt{\varepsilon}}}{1-\sqrt{1-\sqrt{\varepsilon}}}\right) \approx \frac{\varepsilon}{4} \ln \varepsilon$$

To make this process rigourous, one can write $y_1 = \sqrt{\varepsilon} + \delta$. Plugging in, one has $\delta = \varepsilon/2$, continuing this process to solve $y_1 = \cdots + O(\varepsilon^2)$. Similarly, one can compute $y_2 = \ldots + O(\varepsilon^2)$. Keeping the integrand to $O(\varepsilon^2)$ too. One can make sure that the error is $O(\varepsilon^2)$. Then, compute all terms accurately.

4 The problem

It's easy to evaluate $T(E_1)/T(E_0)$ now given the approximation in the last section.