APMA 1941G – HOMEWORK 4

Problem 1: (10 points)

Suppose ϕ has a global max at 0 with $\phi(0) = 0$, $\phi'(0) = 0$, $\phi''(0) = -1$, $\phi'''(0) = 0$. Let $a(x) \equiv 1$ and consider

$$I[\epsilon] = \int_{\mathbb{R}} e^{\frac{\phi(x)}{\epsilon}} dx$$

Show that

$$I[\epsilon] \sim \sqrt{2\pi\epsilon} + \frac{\sqrt{2\pi}}{8}\phi''''(0)\epsilon^{\frac{3}{2}} + o(\epsilon^{\frac{3}{2}})$$

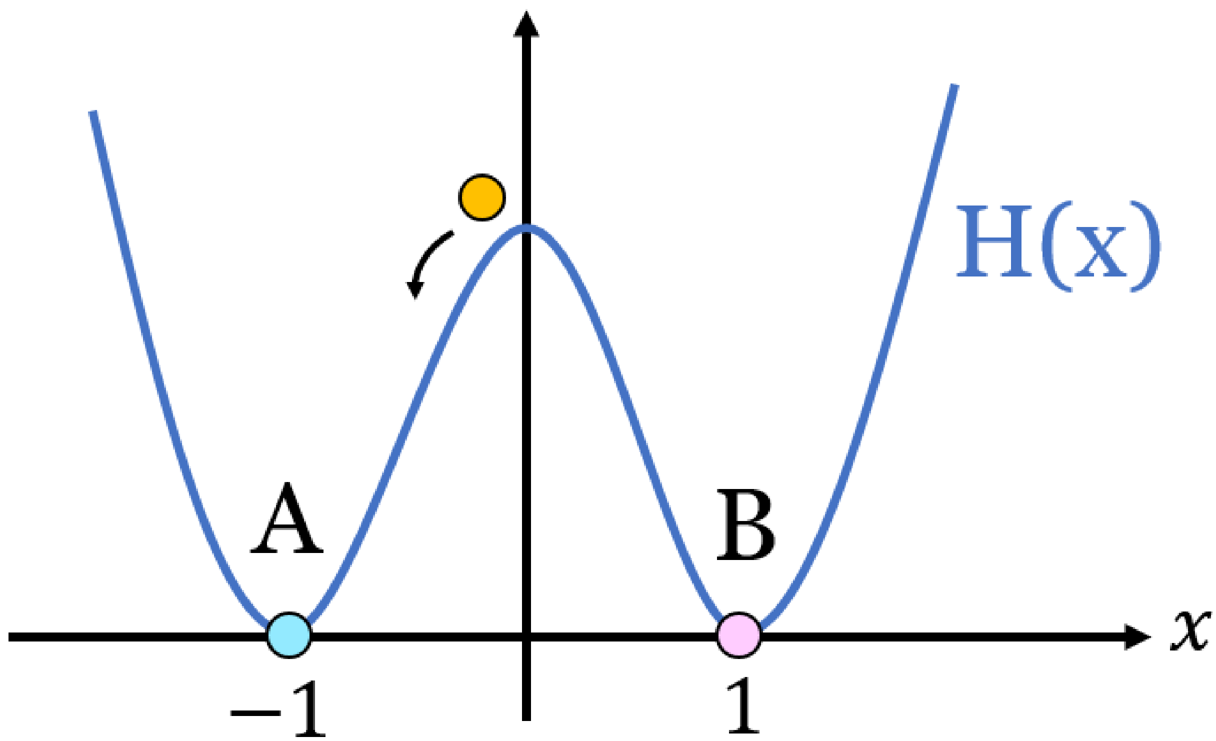
Note: To simplify your task, you may assume that

$$(L_0 a)(0) = a(0)\sqrt{\frac{2\pi}{|\phi''(0)|}} = \sqrt{2\pi}$$

So all you need to calculate is $(L_2 a)(0)$ and $(L_4 a)(0)$. You may also assume that $C_2 = \int_{\mathbb{R}} x^2 e^{-\frac{x^2}{2}} dx = \sqrt{2\pi}$. Of course you may use any results that we derived in lecture.

Problem 2: (10 points, 5 points each)

Suppose that $H = H(x)$ is a double-well potential function, that is, a smooth, even function, with a local min at $x = \pm 1$ with $H(\pm 1) = 0$, a local max at $x = 0$ with $H(0) = 1$, as in the following figure:



Note that Laplace's method is also valid on half-intervals, and in particular it says that, if ϕ has a global maximum at $x = 1$, and for *any* smooth a (not necessarily of compact support), then

$$I[\epsilon] = \int_0^\infty a(x) e^{\frac{\phi(x)}{\epsilon}} dx \sim a(1) e^{\frac{\phi(1)}{\epsilon}} \sqrt{\frac{2\pi\epsilon}{|\phi''(1)|}} + o(\sqrt{\epsilon})$$

(a) Let Z^ϵ be a 'normalizing' constant such that

$$Z^\epsilon \int_{\mathbb{R}} e^{-\frac{H(x)}{\epsilon}} dx = 1$$

Use Laplace's method to show that

$$\frac{1}{Z^{\epsilon}} \sim \frac{2\sqrt{2\pi\epsilon}}{\sqrt{H''(1)}} + o(\sqrt{\epsilon})$$

For sake of simplicity, from now on, let's ignore the remainder term $o(\sqrt{\epsilon})$ and just assume that

$$\frac{1}{Z^{\epsilon}} = \frac{2\sqrt{2\pi\epsilon}}{\sqrt{H''(1)}}$$

(b) Let $\sigma^{\epsilon}(x) = Z^{\epsilon} e^{-\frac{H(x)}{\epsilon}}$ and $\tau^{\epsilon} = \frac{1}{\epsilon} e^{-\frac{1}{\epsilon}}$ and let $\delta = \delta(\epsilon)$ be chosen such that $\delta \to 0$ and $\frac{\delta}{\sqrt{\epsilon}} \to \infty$ as $\epsilon \to 0$. You may think of $\delta = \epsilon^{\frac{1}{4}}$ if you wish.

Use a second-order Taylor expansion of H around 0 (ignore the higher-order terms) as well as the fact that $\int_{\mathbb{R}} e^{-\frac{x^2}{2}} dx = \sqrt{2\pi}$ to show that, as $\epsilon \to 0$

$$\lim_{\epsilon \to 0} \int_{-\delta}^{\delta} \frac{\tau^{\epsilon}}{\sigma^{\epsilon}(x)} dx = \frac{2}{\kappa} \text{ where } \kappa = \frac{\sqrt{|H''(0)|\, H''(1)}}{2\pi}$$

Note: This was one of the problems I had to solve for my thesis. In the context of chemistry, the constant κ is called the reaction-rate constant of the reaction $A \rightleftharpoons B$. This problem demonstrates how the reaction-rate appears in the context of the chemical model. For more info, you can glance at my thesis on my webpage, or in this video:

Video: The PDE that got me the PhD