

Math 379 – Homework 4

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Problem 1: (Muahahaha, yes, I ultimately decided to be evil, but I also simplified this problem a bit so you don't have to suffer *too* much)

This exercise is meant to show you how to explicitly calculate the higher-order terms in the Laplace expansion (in lecture, we did the first term), and to show you how messy things can get in practice!

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

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

Show that

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

Note: To simplify your task, you may assume that

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

(which we showed in lecture), so all you need to calculate are $(L_2 a)(0)$ (this should be quick) 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: 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:

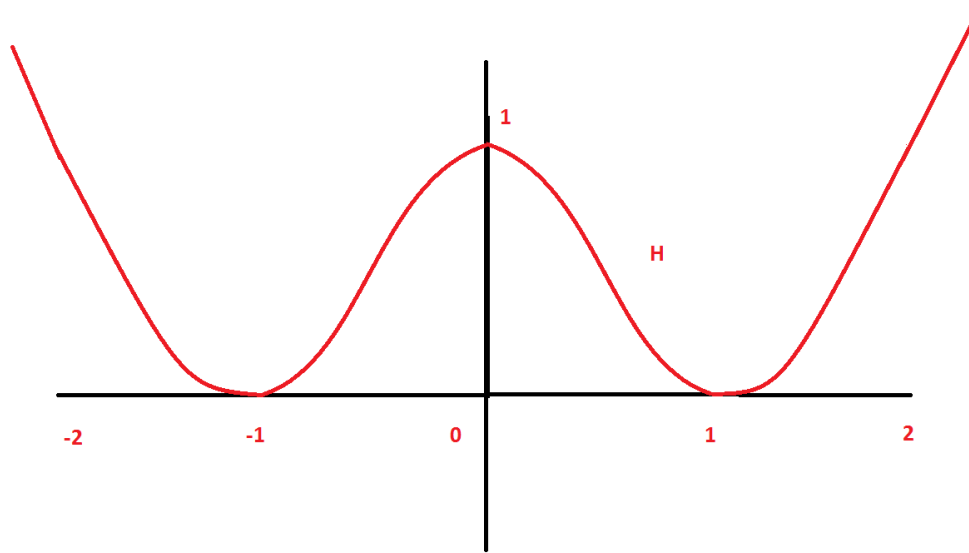


Figure 1: Double-Well Potential Function

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

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

(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 δ (depending on ϵ) be chosen such that $\delta \rightarrow 0$ and $\frac{\delta}{\sqrt{\epsilon}} \rightarrow \infty$ as $\epsilon \rightarrow 0$ (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 $\epsilon \rightarrow 0$

$$\lim_{\epsilon \rightarrow 0} \int_{-\delta}^{\delta} \frac{\tau^\epsilon}{\sigma^\epsilon(x)} dx = \frac{2}{\kappa},$$

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 website!