Appendix D

Laplace's method

Here, Laplace's method of asymptotic evaluation of integrals depending on parameter ς is explained. We follow the line of [36]. For a more detailed justification see [34] or [13].

Consider the integral

$$I(\varsigma) \;=\; \int_a^b e^{-\frac{2V(y)}{\varsigma^2}}\, w(y)\,\mathrm{d}y, \tag{D.1}$$

in which $a, b \in [-\infty, \infty]$, U and w are smooth functions on $\mathbf{R}$, $\varsigma > 0$. The following powerful method for approximating $I(\varsigma)$, $\varsigma \to 0$, goes back to Laplace [26]. According to Laplace, the major contribution to the value of the integral arises from the immediate vicinity of those points of the interval $[a, b]$ at which V assumes its smallest value. Let the minimum of V occur, say, at $y = y_{\min}$. if ς is small, the graph of the integrand has a very sharp peak at $y_{\min}$. It suggests that the overwhelming contribution to the integral comes from the neighbourhood of $y_{\min}$. Accordingly, we replace V and w by the leading terms in their series expansions in $y - y_{\min}$, and then extend the integration limits to $\pm\infty$. The evaluation of the resulting integral yields the required approximation.

We consider two major cases. Suppose first that a is finite, $y_{\min} = a$, $V'(a) > 0$ and $w(a) \neq 0$. Then Laplace's estimation reads as follows

$$\begin{aligned} I(\varsigma) &= \int_a^b e^{-\frac{2V(y)}{\varsigma^2}}\, w(y)\,\mathrm{d}y \simeq \int_a^b e^{-\frac{2}{\varsigma^2}(V(a)+(y-a)V'(a))}\, w(a)\,\mathrm{d}y, \\ &\simeq w(a)\, e^{-\frac{2V(a)}{\varsigma^2}} \int_a^{\infty} e^{-\frac{2}{\varsigma^2}(y-a)V'(a)}\,\mathrm{d}y = \frac{2\varsigma^2 w(a) e^{-\frac{2V(a)}{\varsigma^2}}}{V'(a)}. \end{aligned}$$

The second major case arises when V has a simple minimum at an interior point $y_{\min}$ of (a, b) and $w(y_{\min}) \neq 0$. Then

$$\begin{aligned} I(\varsigma) &= \int_a^b e^{-\frac{2V(y)}{\varsigma^2}} w(y)\,\mathrm{d}y \\ &\simeq \int_a^b e^{-\frac{2}{\varsigma^2}(V(y_{\min})+\frac{1}{2}(y-y_{\min})^2 V''(y_{\min}))} w(y_{\min})\,\mathrm{d}y \\ &\simeq w(y_{\min})\, e^{-\frac{2V(y_{\min})}{\varsigma^2}} \int_{-\infty}^{\infty} e^{-\frac{V''(y_{\min})}{\varsigma^2}(y-y_{\min})^2}\,\mathrm{d}y \\ &= w(y_{\min}) e^{-\frac{2V(y_{\min})}{\varsigma^2}} \sqrt{\frac{\pi\varsigma^2}{V''(y_{\min})}}. \end{aligned}$$

If V has a finite number of minima, we may break up the integral (D.1) into a finite number of integrals so that in each interval V reaches its minimum at one of the end-points and at no other point. Accordingly, we shall assume that V reaches its minimum at $y = a$ and that $V(y) > V(a)$, $a < y \leq b$. Now we precisely formulate the theorem about Laplace's approximation, see [34, Chapters 7,9].

Theorem D.0.4 *Let* $a \in \mathbf{R}$, $b \in \mathbf{R} \cup \{+\infty\}$, $a < b$. *Let* $V : \mathbf{R} \to \mathbf{R}$ *be differentiable, and* $w : \mathbf{R} \to \mathbf{R}$ *or* $\mathbf{C}$ *be measurable.*

Suppose in addition that

(i.) *the minimum of* V *is attained only at* a*;*

(ii.) V' *and* w *are continuous in a neighbourhood of* a*;*

(iii.) *as* $y \downarrow a$,

$$\begin{aligned} V(y) &= V(a) + P(y-a)^{\nu} + \mathcal{O}((y-a)^{\nu+1}), \\ w(y) &= Q(y-a)^{\lambda-1} + \mathcal{O}((y-a)^{\lambda}), \end{aligned}$$

and the first of these relations is differentiable. Here, P*,* ν *and* λ *are positive constants, and* Q *is a real or complex constant.*

(iv.)

$$I(\varsigma) = \int_a^b e^{-\frac{2V(y)}{\varsigma^2}} w(y)\,\mathrm{d}y,$$

converges absolutely throughout its range for all sufficiently small ς*.*

Then

$$I(\varsigma) = \frac{Q}{\nu}\Gamma\left(\frac{\lambda}{\nu}\right)\left(\frac{\varsigma^2}{2P}\right)^{\frac{\lambda}{\nu}} e^{-\frac{2V(a)}{\varsigma^2}}\,(1+\mathcal{O}(\varsigma^{\frac{2}{\nu}})). \tag{D.2}$$

If the asymptotic expansions in ascending powers of $(y-a)$ exist for V and w, the expansion of the integral $I(\varsigma)$ can also be obtained. The first three terms determined in [36]. For our purposes, it is sufficient to use the less exact asymptotics (D.2).

Let us apply Theorem D.0.4 to the double-well potential from Section 2.2.2 that is illustrated in Fig. 2.3 where y_0 denotes the saddle point, m_1 the minimum in the shallow well, and m_2 the minimum in the deep well. The corresponding potential barriers are V^1_{bar} and V^2_{bar}. We want to find the asymptotics of

$$(i.) \qquad I_1(\varsigma) = \int_{-\infty}^{y_0} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y, \tag{D.3}$$

$$(ii.) \qquad I_2(\varsigma) = \int_{y_0}^{\infty} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y, \tag{D.4}$$

$$(iii.) \qquad I_3(\varsigma) = \int_{-\infty}^{\infty} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y. \tag{D.5}$$

We start with the evaluation of $I_1(\varsigma)$. We break the interval $(-\infty, y_0]$ into two intervals $(-\infty, m_1]$ and $[m_1, y_0]$, and note that

$$\begin{aligned} I_1(\varsigma) &= \int_{-\infty}^{y_0} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y = \int_{-\infty}^{m_1} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y + \int_{m_1}^{y_0} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y \\ &= \int_{-m_1}^{\infty} e^{-\frac{2\overline{V}(y)}{\varsigma^2}}\,\mathrm{d}y + \int_{m_1}^{y_0} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y, \end{aligned} \tag{D.6}$$

where $\bar{V}(y) = V(-y)$, $y \in \mathbf{R}$. Both integrals in the last line of (D.6) satisfy the conditions of Theorem D.0.4. We expand V near m_1 and $\bar{V}$ near $-m_1$ to get

$$\begin{aligned} V(y) &= V(m_1) + \frac{\omega_1}{2}(y-m_1)^2 + \mathcal{O}((y-m_1)^3)), \\ \bar{V}(y) &= \bar{V}(-m_1) + \frac{\omega_1}{2}(y+m_1)^2 + \mathcal{O}((y+m_1)^3)), \end{aligned}$$

with $\omega_1 = V''(m_1) = \bar{V}''(-m_1)$. Thus, $P = \omega_1/2$, $\nu = 2$, $\lambda = 1$, $\mathcal{Q} = 1$. A direct application of Theorem D.0.4 yields with $\bar{V}(-m_1) = V(m_1)$

$$\begin{aligned} \int_{-m_1}^{\infty} e^{-\frac{2\bar{V}(y)}{\varsigma^2}}\,\mathrm{d}y &= \frac{\varsigma}{2}\sqrt{\frac{\pi}{\omega_1}}\, e^{-\frac{2V(m_1)}{\varsigma^2}}\,(1+\mathcal{O}(\varsigma)), \\ \int_{m_1}^{y_0} e^{-\frac{2\bar{V}(y)}{\varsigma^2}}\,\mathrm{d}y &= \frac{\varsigma}{2}\sqrt{\frac{\pi}{\omega_1}}\, e^{-\frac{2V(m_1)}{\varsigma^2}}\,(1+\mathcal{O}(\varsigma)), \end{aligned}$$

and, consequently,

$$I_1(\varsigma) = \int_{-\infty}^{y_0} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y = \varsigma\sqrt{\frac{\pi}{\omega_1}}\, e^{-\frac{2V(m_1)}{\varsigma^2}}\,(1+\mathcal{O}(\varsigma)).$$

Analogously, one evaluates the integral

$$\begin{aligned} I_2(\varsigma) &= \int_{y_0}^{\infty} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y = \int_{y_0}^{m_2} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y + \int_{m_2}^{\infty} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y \\ &= \int_{-m_2}^{-y_0} e^{-\frac{2\bar{V}(y)}{\varsigma^2}}\,\mathrm{d}y + \int_{m_2}^{\infty} e^{-\frac{2V(y)}{\varsigma^2}}\,\mathrm{d}y = \varsigma\sqrt{\frac{\pi}{\omega_1}}\,e^{-\frac{2V(m_2)}{\varsigma^2}}\,(1+\mathcal{O}(\varsigma)). \end{aligned}$$

Without loss of generality we assume $V(m_2) = \min(V(m_1), V(m_2))$ and obtain for the asymptotics of (D.5):

$$I_3(\varsigma) = I_1(\varsigma) + I_2(\varsigma) = \varsigma\sqrt{\frac{\pi}{\omega_1}}\,e^{-\frac{2V(m_2)}{\varsigma^2}}\,(1+\mathcal{O}(\varsigma)).$$