

Appendix E

Second Eigenvector of \mathcal{L}^ϵ : Illustrative Example

Here, we refer to the last paragraph of Section 3.5.4 and compute the second eigenvector of the full dynamics' generator \mathcal{L}^ϵ in order to numerically compare the asymptotic result (3.75). To this end, we have chosen the potential $V = V(x, y)$ as

$$V(x, y) = 5(y^2 - 1)^2 + 1.25(y - x/2)^2. \quad (\text{E.1})$$

The potential is shown in Figure E.1. The metastable decomposition for fixed x is approximately given by $B_x^{(1)} = \{(x, y) : y \in \mathbf{R}^-\}$ and $B_x^{(2)} = \{(x, y) : y \in \mathbf{R}^+\}$. For the computation of the eigenvector, we choose $\epsilon = 0.005$ fixed and increase the inverse temperature β . Concerning the structure of the second eigenvector u^ϵ , this can be considered equivalent to increasing the potential barrier in the direction of the fast variable y . For small values of β , the eigenvector $u^\epsilon(x, \cdot)$ is independent of the fast variable y , but clearly depends on x . The pictures seem to confirm the validity of the asymptotic strategy to derive u^ϵ that is outlined in the last paragraph of Section 3.5.4. For small values of β we obtain

$$u^\epsilon(x, y) \approx a_1(x) \mathbf{1}_{B_x^{(1)}}(y) + a_2(x) \mathbf{1}_{B_x^{(2)}}(y),$$

whereas for $\beta = 8.5$ we approximately have

$$u^\epsilon(x, y) \approx a_1 \mathbf{1}_{B^{(1)}}(x, y) + a_2 \mathbf{1}_{B^{(2)}}(x, y),$$

where a_1 and a_2 now are independent of x . The pictures also reveal that the simple averaging procedure is inappropriate for $\beta \geq 2.5$.

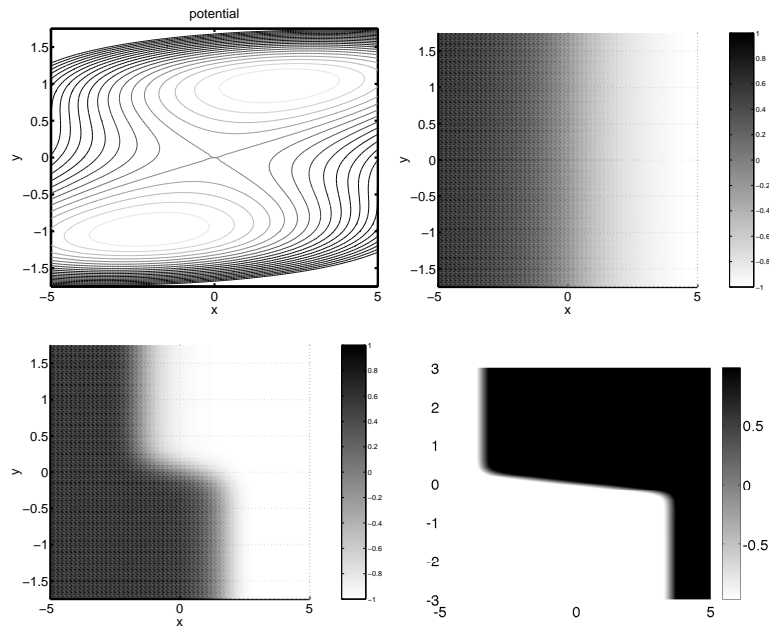


Figure E.1: Second eigenvector of \mathcal{L}^ϵ corresponding to the potential V in (E.1) for $\epsilon = 0.005$ and $\beta = 1.0$ (right, top), $\beta = 2.5$ (bottom, left) and $\beta = 8.5$ (bottom, right).