Asymptotics for scaled Kramers-Smoluchowski equations

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Abstract

We offer fairly simple and direct proofs of the asymptotics for the scaled Kramers-Smoluchowski equation in both one and higher dimensions. For the latter, we invoke the sharp asymptotic capacity asymptotics of Bovier–Eckhoff–Gayrard–Klein [B-E-G-K].

1 Introduction

The simplest one-dimensional version of the scaled Kramers-Smoluchowski PDE has the form

$$\rho_t^\epsilon = \left(\rho_\xi^\epsilon + \epsilon^{-2}\rho^\epsilon\Phi'\right)_\xi \tag{1.1}$$

for the chemical density $\rho^\epsilon = \rho^\epsilon(\xi, t)$, where $\Phi = \Phi(\xi)$ is an even chemical potential having two wells, say at the points ± 1. Formal asymptotics suggest that if the time t is rescaled by an appropriate factor τ_ϵ, then

$$\rho^\epsilon \rightharpoonup \alpha\delta_{-1} + \beta\delta_1$$

as $\epsilon \to 0$, where $\alpha = \alpha(t)$ and $\beta = \beta(t)$ solve the system of ODE

$$\begin{cases} \alpha' = \kappa(\beta - \alpha) \\ \beta' = \kappa(\alpha - \beta) \end{cases}$$

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for an appropriate Kramers rate constant κ, computed in terms of Φ. Consult Berglund [B] for much more about Kramers' formula.

This asymptotic problem has in recent years been treated by several teams of authors. An interesting paper by Peletier-Savare-Veneroni [P-S-V1] (rewritten as [P-S-V2]) provides rigorous proofs, allowing also for diffusion effects in other spatial variables x. Their approach invokes ideas of Γ-convergence. Later Herrmann and Niethammer [H-N] pointed out that the Γ-convergence perspective was not really needed, and instead interpreted (1.1) as a gradient flow on the Wasserstein space of probability measures. Their proofs in fact do not really use the Wasserstein viewpoint very much, relying instead on a Raleigh-type dissipation functional. S. Arnrich et al in [A-M-P-S-V] revisit this problem, providing a complete interpretation of the dynamics as providing a curve of maximal slope for a Wasserstein gradient flow.

In this paper we provide an even greater simplification, requiring nothing abstract at all. We instead just build a simple test function (see (2.27)), integrate by parts and use some fairly easy estimates. (Our auxiliary function ϕ^ϵ is however strongly related to the analysis in Section 5.3 of [P-S-V2] on "minimal transition costs".) The direct technique is robust, and generalizes, with some difficulties, to higher dimensions for the chemical potential variable ξ. In this setting we need the sharp asymptotic capacity asymptotics of Bovier–Eckhoff–Gayrard–Klein [B-E-G-K].

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2 Kramers-Smoluchowski in one dimension

We assume that $\Phi : \mathbb{R} \to \mathbb{R}$, $\Phi = \Phi(\xi)$, is a smooth, nonnegative and even double-well potential function, with a local maximum at 0 and local minima at ± 1, normalized so that $\Phi(0) = 1$, $\Phi(\pm 1) = 0$, $\Phi(\pm 2) = 1$. We suppose also that $\Phi''(0) < 0$ and $\Phi''(\pm 1) > 0$ and that Φ is strictly decreasing on $(0, 1)$ and strictly increasing on $(1, \infty)$. Assume as well that Φ grows at least linearly as $|\xi| \to \infty$. Then Φ has the W shape drawn in the illustration.

2.1 Kramers-Smoluchowski equation. Define

$$\sigma^\epsilon = \frac{e^{\frac{-\Phi}{\epsilon^2}}}{Z_\epsilon}, \tag{2.1}$$

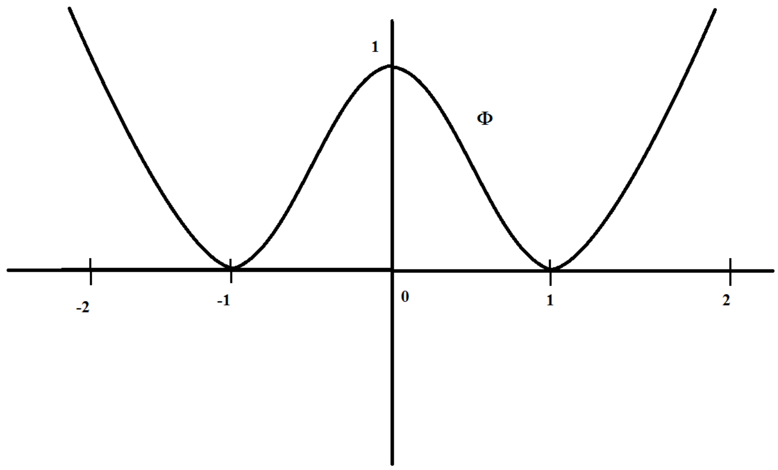

Figure 1: Graph of Φ

the normalization constant Z_ϵ chosen so that $\int_{\mathbb{R}} \sigma^\epsilon \, d\xi = 1$. We also introduce the scaling factor

$$\tau_\epsilon := \frac{1}{\epsilon^2} e^{-\frac{1}{\epsilon^2}}, \tag{2.2}$$

which, as pointed out in [P-S-V1], provides the correct dilation in time for a nontrivial asymptotic limit. As in the papers cited in the introduction, a key point will be showing that the rate constant in the linear reaction-diffusion system (2.26) derived later is

$$\kappa := \frac{\sqrt{|\Phi''(0)|\, \Phi''(\pm 1)}}{2\pi}. \tag{2.3}$$

We study solutions $\rho^\epsilon = \rho^\epsilon(x, \xi, t)$ of this initial-value problem for the scaled **Kramers-Smoluchowski equation**:

$$\begin{cases} \tau_\epsilon \left(\rho^\epsilon_t - a\Delta_x \rho^\epsilon\right) = \left(\rho^\epsilon_\xi + \epsilon^{-2} \rho^\epsilon \Phi'\right)_\xi & \text{in } U \times \mathbb{R} \times [0, T] \\ \frac{\partial \rho^\epsilon}{\partial \nu} = 0 & \text{on } \partial U \times \mathbb{R} \times [0, T] \\ \rho^\epsilon = \rho^\epsilon_0 & \text{on } U \times \mathbb{R} \times \{t = 0\}, \end{cases} \tag{2.4}$$

where U is a bounded, smooth domain in $\mathbb{R}^n$, $\frac{\partial \rho^\epsilon}{\partial \nu} = D_x \rho^\epsilon \cdot \nu$ is the outward normal derivative along ∂U, and $\rho^\epsilon_0 = \rho^\epsilon_0(x, \xi) \geq 0$ is given. We are given also the smooth and bounded function $a = a(\xi)$, satisfying

$$a \geq a_0 > 0 \tag{2.5}$$

for some constant a_0. We hereafter write $x \in U$, $\xi \in \mathbb{R}$, $0 \leq t \leq T$.

Now define

$$u^\epsilon := \frac{\rho^\epsilon}{\sigma^\epsilon}; \tag{2.6}$$

so that $u^\epsilon = u^\epsilon(x, \xi, t)$. Then (2.4) transforms into

$$\begin{cases} \tau_\epsilon \sigma^\epsilon (u^\epsilon_t - a\Delta_x u^\epsilon) = \left(\sigma^\epsilon u^\epsilon_\xi\right)_\xi & \text{in } U \times \mathbb{R} \times [0,T] \\ \frac{\partial u^\epsilon}{\partial \nu} = 0 & \text{on } \partial U \times \mathbb{R} \times [0,T] \\ u^\epsilon = u^\epsilon_0 & \text{on } U \times \mathbb{R} \times \{t = 0\} \end{cases} \tag{2.7}$$

for $u^\epsilon_0 := \frac{\rho^\epsilon_0}{\sigma^\epsilon}$. The task is to understand the limit of ρ^ϵ and u^ϵ as $\epsilon \to 0$.

2.2 Elementary estimates. We hereafter assume concerning the initial data $u^\epsilon_0 = u^\epsilon_0(x, \xi)$ that

$$0 \leq u^\epsilon_0 \leq C \tag{2.8}$$

for some constant C and

$$\int_{\mathbb{R}} \int_U (|u^\epsilon_0|^2 + |D_x u^\epsilon_0|^2 + \tfrac{1}{\tau_\epsilon} \left|u^\epsilon_{0,\xi}\right|^2) \sigma^\epsilon \, dx d\xi < \infty. \tag{2.9}$$

We suppose in addition that as $\epsilon \to 0$

$$\begin{cases} u^\epsilon_0 \to 2\alpha_0 & \text{locally uniformly on } \bar{U} \times \mathbb{R}_- \\ u^\epsilon_0 \to 2\beta_0 & \text{locally uniformly on } \bar{U} \times \mathbb{R}_+, \end{cases} \tag{2.10}$$

where $\alpha_0 = \alpha_0(x)$ and $\beta_0 = \beta_0(x)$ are smooth and $\mathbb{R}_\pm = \{\pm\xi > 0\}$.

Lemma 2.1. *We have the estimates*

$$0 \leq u^\epsilon \leq C \tag{2.11}$$

and

$$\sup_{0 \leq t \leq T} \int_{\mathbb{R}} \int_U (|u^\epsilon|^2 + |D_x u^\epsilon|^2 + \tfrac{1}{\tau_\epsilon} \left|u^\epsilon_\xi\right|^2) \sigma^\epsilon \, dx d\xi + \int_0^T \int_{\mathbb{R}} \int_U |u^\epsilon_t|^2 \, \sigma^\epsilon \, dx \, d\xi dt \leq C \tag{2.12}$$

for a constant C independent of ϵ.

Proof. The maximum principle and (2.8) imply (2.11). Next, multiply (2.7) by u^ϵ and integrate in time, recalling (2.5) and (2.9) to derive the bound

$$\sup_{0\le t\le T}\int_{\mathbb{R}}\int_U |u^\epsilon|^2\,\sigma^\epsilon\,dx\,d\xi+\int_0^T\int_{\mathbb{R}}\int_U(|D_x u^\epsilon|^2+\tfrac{1}{\tau_\epsilon}\left|u^\epsilon_\xi\right|^2)\sigma^\epsilon\,dx\,d\xi dt\le C.$$

Finally, multiply (2.7) by u^ϵ_t and again integrate, using (2.5), (2.9) once more to estimate

$$\sup_{0\le t\le T}\int_{\mathbb{R}}\int_U(|D_x u^\epsilon|^2+\tfrac{1}{\tau_\epsilon}\left|u^\epsilon_\xi\right|^2)\sigma^\epsilon\,dxd\xi+\int_0^T\int_{\mathbb{R}}\int_U|u^\epsilon_t|^2\,\sigma^\epsilon\,dx\,d\xi dt\le C.$$

□

2.3 Asymptotic estimates. We next recall Laplace's asymptotics (see for instance Bender–Orszag [B-O]):

Lemma 2.2. *If $f=f(\xi)$ is a smooth function on $[a,b]$, if $\xi_0\in(a,b)$ is the unique maximum point and if $f''(\xi_0)<0$, then*

$$\int_a^b e^{\frac{f}{\epsilon^2}}\,d\xi=e^{\frac{f(\xi_0)}{\epsilon^2}}\left(\frac{2\pi\epsilon^2}{-f''(\xi_0)}\right)^{\frac12}(1+o(1))\qquad \textit{as } \epsilon\to 0. \tag{2.13}$$

Now put

$$\gamma=\gamma(\epsilon)=\epsilon^{\frac34}. \tag{2.14}$$

and define the regions

$$I_\gamma:=(-1-\gamma,-1+\gamma)\cup(1-\gamma,1+\gamma)$$
$$J_\gamma:=(-2+\gamma,-\gamma)\cup(\gamma,2-\gamma),\;\;K:=(-3,-\tfrac52)\cup(\tfrac52,3).$$

We recall now some useful facts from Herrmann–Niethammer [H-N] and Peletier-Savare-Veneroni [P-S-V1].

Lemma 2.3. (i) *We have*

$$Z_\epsilon=\left(\frac{8\pi\epsilon^2}{\Phi''(1)}\right)^{\frac12}(1+o(1))\qquad \textit{as } \epsilon\to 0. \tag{2.15}$$

(ii) *Furthermore,*

$$\int\limits_{\mathbb{R}-I_\gamma}\sigma^\epsilon\,d\xi\to 0,\;\int\limits_{J_\gamma}\frac{\tau_\epsilon}{\sigma^\epsilon}\,d\xi\to 0,\;\int_K\frac{\sigma^\epsilon}{\tau_\epsilon}\,d\xi\to 0 \tag{2.16}$$

and

$$\int_{\pm 1-\gamma}^{\pm 1+\gamma} \sigma^\epsilon \, d\xi \to \frac{1}{2}, \; \int_{-\gamma}^{\gamma} \frac{\tau_\epsilon}{\sigma^\epsilon} \, d\xi \to \frac{2}{\kappa}. \tag{2.17}$$

Proof. 1. Since Φ is even and $\Phi(1) = 0$, Lemma 2.2 implies

$$Z_\epsilon = \int_{\mathbb{R}} e^{-\frac{\Phi}{\epsilon^2}} \, d\xi = 2 \int_0^\infty e^{-\frac{\Phi}{\epsilon^2}} \, d\xi = 2 \left(\frac{2\pi\epsilon^2}{\Phi''(1)} \right)^{\frac{1}{2}} (1 + o(1)).$$

2. The limits (2.16) are elementary, as $\lim_{\epsilon\to 0} \frac{e^{-\frac{\gamma^2}{\epsilon^2}}}{\epsilon^2} = 0$; and the first limit in (2.17) follows. Since

$$\Phi(\xi) = 1 + \frac{\Phi''(0)}{2}\xi^2 + O(|\xi|^3) \quad \text{as } \xi \to 0$$

and $\lim_{\epsilon\to 0} \frac{\gamma^3}{\epsilon^2} = 0$, $\lim_{\epsilon\to 0} \frac{\gamma}{\epsilon} = \infty$, we have

$$\begin{aligned} \int_{-\gamma}^{\gamma} \frac{\tau_\epsilon}{\sigma^\epsilon} \, d\xi =& \frac{Z_\epsilon}{\epsilon^2} \int_{-\gamma}^{\gamma} e^{\frac{\Phi''(0)}{2} \frac{(\xi^2 + O(|\xi|^3))}{\epsilon^2}} \, d\xi \\ =& \left(\frac{8\pi}{\Phi''(1)} \right)^{\frac{1}{2}} \int_{-\frac{\gamma}{\epsilon}}^{\frac{\gamma}{\epsilon}} e^{-\frac{|\Phi''(0)|}{2}\xi^2} \, d\xi (1 + o(1)) \\ \to& \left(\frac{8\pi}{\Phi''(1)} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{|\Phi''(0)|}{2}\xi^2} \, d\xi = \frac{4\pi}{\sqrt{|\Phi''(0)| \, \Phi''(1)}} = \frac{2}{\kappa}. \end{aligned}$$

□

2.4 Compactness and convergence. We henceforth write $U_T := U \times (0, T)$.

Lemma 2.4. (i) *There exists a subsequence* $\epsilon = \epsilon_k \to 0$ *and functions* $\alpha, \beta \in H^1(U_T)$ *such that*

$$\int_{-1-\gamma}^{-1+\gamma} \rho^\epsilon \, d\xi \to \alpha, \; \int_{1-\gamma}^{1+\gamma} \rho^\epsilon \, d\xi \to \beta \tag{2.18}$$

in $L^2(U_T)$ *and*

$$\sup_{0\le t\le T} \int_{\mathbb{R}-I_\gamma} \int_U |\rho^\epsilon| \, dx \, d\xi \to 0. \tag{2.19}$$

(ii) *In addition,*

$$\int_{-1-\gamma}^{-1+\gamma} \rho_t^\epsilon \, d\xi \rightharpoonup \alpha_t, \ \int_{1-\gamma}^{1+\gamma} \rho_t^\epsilon \, d\xi \rightharpoonup \beta_t \tag{2.20}$$

and

$$\int_{-1-\gamma}^{-1+\gamma} D_x\rho^\epsilon \, d\xi \rightharpoonup D_x\alpha, \ \int_{1-\gamma}^{1+\gamma} D_x\rho^\epsilon \, d\xi \rightharpoonup D_x\beta \tag{2.21}$$

weakly in $L^2(U_T)$*, with*

$$\int_{\mathbb{R}-I_\gamma} \int_U |\rho_t^\epsilon| \, dx \, d\xi \to 0 \tag{2.22}$$

strongly in $L^2(0,T)$ *and*

$$\sup_{0\le t\le T} \int_{\mathbb{R}-I_\gamma} \int_U |D_x\rho^\epsilon| \, dx \, d\xi \to 0. \tag{2.23}$$

(iii) *Also, for each time* $0 \le t \le T$ *and almost every* $x \in U$*, we have*

$$\begin{cases} u^\epsilon \to 2\alpha & \text{locally uniformly for } -2 < \xi < 0 \\ u^\epsilon \to 2\beta & \text{locally uniformly for } \ 0 < \xi < 2 \end{cases} \tag{2.24}$$

as $\epsilon \to 0$.

Proof. 1. Since $\rho^\epsilon = u^\epsilon\sigma^\epsilon$, we can use (2.12) and (2.16) to deduce that

$$\sup_{0\le t\le T} \int_{\mathbb{R}-I_\gamma} \int_U |\rho^\epsilon| \, dx \, d\xi \\ \le C \sup_{0\le t\le T} \left(\int_{\mathbb{R}} \int_U |u^\epsilon|^2 \, \sigma^\epsilon dx \, d\xi \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}-I_\gamma} \sigma^\epsilon \, d\xi \right)^{\frac{1}{2}} \to 0.$$

Likewise, (2.22) and (2.23) hold.

2. Now define the functions

$$\alpha_\epsilon(x,t) := \int_{-1-\gamma}^{-1+\gamma} \rho^\epsilon(x,\xi,t) \, d\xi, \quad \beta_\epsilon(x,t) := \int_{1-\gamma}^{1+\gamma} \rho^\epsilon(x,\xi,t) \, d\xi.$$

Then (2.12) implies

$$\int_0^T \int_U |\alpha_\epsilon|^2 + |\alpha_{\epsilon,t}|^2 + |D_x \alpha_\epsilon|^2 \, dxdt \le C$$
$$\int_0^T \int_U |\beta_\epsilon|^2 + |\beta_{\epsilon,t}|^2 + |D_x \beta_\epsilon|^2 \, dxdt \le C.$$

Therefore we can extract a subsequence $\epsilon = \epsilon_k \to 0$, such that $\alpha_\epsilon \rightharpoonup \alpha$, $\beta_\epsilon \rightharpoonup \beta$ weakly in $H^1(U_T)$ and strongly in $L^2(U_T)$, as $\epsilon = \epsilon_k \to 0$.

3. If $0 < a < b < 2$, then (2.12) and (2.16) show that

$$\int_a^b \int_U \left| u_\xi^\epsilon \right| dx \, d\xi \le \left(\int_a^b \int_U \frac{\sigma^\epsilon}{\tau_\epsilon} \left| u_\xi^\epsilon \right|^2 dx \, d\xi \right)^{\frac{1}{2}} \left(\int_{J_\gamma} \frac{\tau_\epsilon}{\sigma^\epsilon} \, d\xi \right)^{\frac{1}{2}} \to 0.$$

Hence for each time t,

$$\int_U \operatorname{osc}_{a \le \xi \le b} u^\epsilon \, dx \to 0;$$

osc denoting oscillation in the variable ξ. So for each $0 \le t \le T$ and almost every $x \in U$, u^ϵ converges for $0 < \xi < 2$ to a function $u = u(x,t)$. However, since

$$\alpha_\epsilon = \int_{-1-\gamma}^{-1+\gamma} \sigma^\epsilon u^\epsilon \, d\xi,$$

the first limit in (2.17) implies that $u = 2\alpha$ if $0 < \xi < 2$. The other case follows similarly. □

2.5 Derivation of the limit reaction-diffusion PDE. The interesting issue is finding the limit PDE for α and β:

Theorem 2.5. *For all $0 \le t \le T$, we have*

$$\rho^\epsilon \rightharpoonup \alpha\delta_{-1} + \beta\delta_1, \tag{2.25}$$

where the smooth functions $\alpha = \alpha(x,t)$ and $\beta = \beta(x,t)$ solve the linear reaction-diffusion system

$$\begin{cases} \alpha_t - a^- \Delta\alpha = \kappa(\beta - \alpha) & \text{in } U_T \\ \beta_t - a^+ \Delta\beta = \kappa(\alpha - \beta) & \text{in } U_T \\ \frac{\partial\alpha}{\partial\nu} = \frac{\partial\beta}{\partial\nu} = 0 & \text{on } \partial U \times [0,T] \\ \alpha = \alpha_0, \ \beta = \beta_0 & \text{on } U \times \{t=0\}, \end{cases} \tag{2.26}$$

for the diffusion constants $a^\pm := a(\pm 1)$.

The initial data are given by (2.10).

Proof. 1. Select any test function $\zeta \in C^\infty(\bar{U}_T)$, $\zeta = \zeta(x,t)$. Let $\psi = \psi(\xi)$ be a smooth function supported on $[-3,3]$ such that $0 \le \psi \le 1$ and $\psi \equiv 1$ on $\left[-\frac{5}{2}, \frac{5}{2}\right]$. Define also

$$\phi^\epsilon(\xi) := \int_0^{\Lambda(\xi)} \frac{\tau_\epsilon}{\sigma^\epsilon(\eta)}\, d\eta, \tag{2.27}$$

where $\Lambda(s) = s$ if $-\frac{3}{2} < s < \frac{3}{2}$ and $\Lambda(s) = \pm\frac{3}{2}$ if $\pm s \ge \frac{3}{2}$. According to (2.16) and (2.17), ϕ^ϵ is bounded and

$$\phi^\epsilon \to \begin{cases} -\frac{1}{\kappa} & \text{uniformly on } (-\frac{3}{2}, -\frac{1}{2}) \\ \frac{1}{\kappa} & \text{uniformly on } (\frac{1}{2}, \frac{3}{2}). \end{cases} \tag{2.28}$$

2. Multiplying (2.7) by $\psi\phi^\epsilon\zeta$ and integrating by parts, we get

$$\int_0^T\int_U\int_{-3}^3 \psi\phi^\epsilon\zeta u_t^\epsilon\sigma^\epsilon\, d\xi dx dt + \int_0^T\int_U\int_{-3}^3 \psi\phi^\epsilon a D_x u^\epsilon \cdot D_x\zeta\sigma^\epsilon\, d\xi dx dt$$
$$= -\int_0^T\int_U\int_{-3}^3 (\psi\phi^\epsilon)_\xi \zeta \frac{\sigma^\epsilon}{\tau_\epsilon} u_\xi^\epsilon\, d\xi dx dt. \tag{2.29}$$

Now (2.22) implies

$$\left|\int_0^T\int_U\int_{\mathbb{R}-I_\gamma} \psi\phi^\epsilon\zeta\rho_t^\epsilon\, d\xi dx dt\right| \le C\int_0^T\int_U\int_{\mathbb{R}-I_\gamma} |\rho_t^\epsilon|\, d\xi dx dt \to 0$$

Note that $\psi \equiv 1$ on I_γ and remember (2.20), (2.28):

$$\int_0^T\int_U\int_{-1-\gamma}^{-1+\gamma} \psi\phi^\epsilon\zeta\rho_t^\epsilon\, d\xi dx dt = \int_0^T\int_U\left(\int_{-1-\gamma}^{-1+\gamma} \phi^\epsilon\rho_t^\epsilon\, d\xi\right)\zeta\, dx dt$$
$$\to -\frac{1}{\kappa}\int_0^T\int_U \alpha_t\zeta\, dx dt.$$

Likewise,

$$\int_0^T\int_U\int_{1-\gamma}^{1+\gamma} \psi\phi^\epsilon\zeta\rho_t^\epsilon\, d\xi dx dt \to \frac{1}{\kappa}\int_0^T\int_U \beta_t\zeta\, dx dt.$$

Consequently, since $u_t^\epsilon\sigma^\epsilon = \rho_t^\epsilon$,

$$\lim_{\epsilon\to 0}\int_0^T\int_U\int_{-3}^3 \psi\phi^\epsilon u_t^\epsilon\sigma^\epsilon\, d\xi dx dt = \frac{1}{\kappa}\int_0^T\int_U (\beta_t - \alpha_t)\zeta\, dx dt. \tag{2.30}$$

We similarly show using (2.21) that

$$\lim_{\epsilon\to 0}\int_0^T\int_U\int_{-3}^3 \psi\phi^\epsilon a D_x u^\epsilon \cdot D_x\zeta\sigma^\epsilon\, d\xi dx dt$$
$$= \frac{1}{\kappa}\int_0^T\int_U (a^+ D_x\beta - a^- D_x\alpha)\cdot D_x\zeta\, dxdt. \quad (2.31)$$

3. We write the last term in (2.29) as

$$\int_0^T\int_U\int_{-3}^3 \psi\phi^\epsilon_\xi\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}u^\epsilon_\xi\, d\xi dxdt + \int_0^T\int_U\int_{-3}^3 \psi_\xi\phi^\epsilon\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}u^\epsilon_\xi\, d\xi dxdt.$$

Since $\phi^\epsilon_\xi = \frac{\tau_\epsilon}{\sigma^\epsilon}$ if $-\frac{3}{2} < \xi < \frac{3}{2}$ and is zero otherwise,

$$\begin{aligned}\int_0^T\int_U\int_{-3}^3 \psi\phi^\epsilon_\xi\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}u^\epsilon_\xi\, d\xi dxdt &= \int_0^T\int_U\int_{-\frac{3}{2}}^{\frac{3}{2}} \zeta u^\epsilon_\xi\, d\xi dxdt \\ &= \int_0^T\int_U (u^\epsilon\left(x,\tfrac{3}{2},t\right) - u^\epsilon\left(x,-\tfrac{3}{2},t\right))\zeta\, dxdt \\ &\to 2\int_0^T\int_U (\beta-\alpha)\zeta\, dxdt,\end{aligned}$$

according to (2.24). In addition, (2.12) and (2.16) give

$$\left|\int_0^T\int_U\int_{-3}^3 \psi_\xi\phi^\epsilon\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}u^\epsilon_\xi\, d\xi dxdt\right|$$
$$\leq C\left(\int_0^T\int_U\int_{\mathbb{R}} \left|u^\epsilon_\xi\right|^2\frac{\sigma^\epsilon}{\tau_\epsilon} d\xi dxdt\right)^{\frac{1}{2}}\left(\int_K \frac{\sigma^\epsilon}{\tau_\epsilon}\, d\xi\right)^{\frac{1}{2}} \to 0.$$

Hence

$$\lim_{\epsilon\to 0}\int_0^T\int_U\int_{-3}^3 (\psi\phi^\epsilon)_\xi\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}u^\epsilon_\xi\, d\xi dxdt = 2\int_0^T\int_U(\beta-\alpha)\zeta\, dxdt. \quad (2.32)$$

4. Letting $\epsilon\to 0$, we conclude from (2.29)–(2.32) that

$$\int_0^T\int_U(\beta_t-\alpha_t)\zeta\, dxdt + \int_0^T\int_U (a^+ D_x\beta - a^- D_x\alpha)\cdot D_x\zeta\, dxdt$$
$$= -2\kappa\int_0^T\int_U(\beta-\alpha)\zeta\, dxdt. \quad (2.33)$$

It follows that

$$\beta_t - \alpha_t - (a^+\Delta\beta - a^-\Delta\alpha) = 2\kappa(\alpha - \beta). \tag{2.34}$$

in the sense of distributions.

5. We need another functional relation between α and β. To get this, we multiply (2.7) by $\psi\zeta$ and again integrate by parts:

$$\int_0^T\int_U\int_{-3}^3 \psi\zeta u_t^\epsilon \sigma^\epsilon \, d\xi dx dt + \int_0^T\int_U\int_{-3}^3 \psi a D_x u^\epsilon \cdot D_x\zeta \sigma^\epsilon \, d\xi dx dt$$
$$= -\int_0^T\int_U\int_{-3}^3 \psi_\xi \zeta \frac{\sigma^\epsilon}{\tau_\epsilon} u_\xi^\epsilon \, d\xi dx dt.$$

Passing to limits as $\epsilon \to 0$ gives

$$\int_0^T\int_U (\beta_t + \alpha_t)\zeta \, dx dt + \int_0^T\int_U (a^+ D_x\beta + a^- D_x\alpha)\cdot D_x\zeta \, dx dt = 0. \tag{2.35}$$

Consequently,

$$\beta_t + \alpha_t - (a^+\Delta\beta + a^-\Delta\alpha) = 0 \tag{2.36}$$

as distributions.

Simultaneously solving (2.34) and (2.36), we deduce that

$$\alpha_t - a^-\Delta\alpha = \kappa(\beta - \alpha), \;\; \beta_t - a^+\Delta\beta = \kappa(\alpha - \beta)$$

in the weak sense. In addition, since the integral identities (2.33) and (2.35) are valid even if ζ does not vanish on $\partial U \times [0, T]$, we have

$$a^+\frac{\partial\beta}{\partial\nu} - a^-\frac{\partial\alpha}{\partial\nu} = 0, \;\; a^+\frac{\partial\beta}{\partial\nu} + a^-\frac{\partial\alpha}{\partial\nu} = 0,$$

and thus

$$\frac{\partial\beta}{\partial\nu} = 0, \;\; \frac{\partial\alpha}{\partial\nu} = 0$$

on $\partial U \times [0, T]$ in the weak sense. Regularity theory for parabolic PDE (see for instance Lieberman [L]) implies that α and β are in fact smooth. □

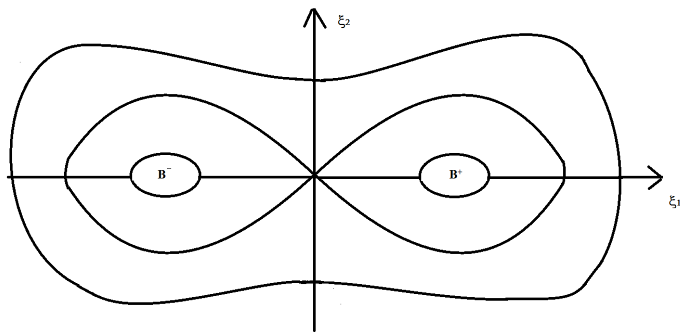

Figure 2: Level sets of Φ

3 Generalization to higher dimensions

Our methods are robust enough that we can tackle as well some higher dimensional generalizations, for which the variable ξ lies in $\mathbb{R}^m$. For simplicity, we assume that the chemical potential $\Phi : \mathbb{R}^m \to \mathbb{R}$ is smooth, nonnegative and even in the first variable ξ_1.

We suppose also that Φ has two wells, at the points

$$e^{\pm} := (\pm 1, 0, \dots, 0),$$

connected by a single nondegenerate saddle point at the origin, normalized so that $\Phi(0) = 1$, $\Phi(e^{\pm}) = 0$. We assume furthermore that Φ grows at least linearly as $|\xi| \to \infty$. In addition, we require that $\det D^2\Phi(e^{\pm}) \neq 0$, $\det D^2\Phi(0) \neq 0$, and that $D^2\Phi(0)$ is diagonal, with eigenvalues

$$\lambda_1(0) < 0 < \lambda_2(0) \leq \cdots \leq \lambda_m(0).$$

The Kramers rate constant will turn out to be

$$\kappa := \frac{|\lambda_1(0)|}{2\pi} \frac{\sqrt{|\det D^2\Phi(e^{\pm})|}}{\sqrt{|\det D^2\Phi(0)|}}; \tag{3.1}$$

this agrees with (2.3) when $m = 1$.

3.1 Extending the Kramers-Smoluchowski equation. The higher dimensional analog of (2.4) reads

$$\begin{cases} \tau_\epsilon \left(\rho^\epsilon_t - a\Delta_x \rho^\epsilon\right) = \operatorname{div}_\xi(D_\xi \rho^\epsilon + \epsilon^{-2}\rho^\epsilon D\Phi) & \text{in } U \times \mathbb{R}^m \times [0,T] \\ \frac{\partial \rho^\epsilon}{\partial \nu} = 0 & \text{on } \partial U \times \mathbb{R}^m \times [0,T] \\ \rho^\epsilon = \rho^\epsilon_0 & \text{on } U \times \mathbb{R}^m \times \{t=0\} \end{cases} \tag{3.2}$$

for

$$\tau_\epsilon := \frac{1}{\epsilon^2} e^{-\frac{1}{\epsilon^2}}. \tag{3.3}$$

As before, set

$$\sigma^\epsilon := \frac{e^{\frac{-\Phi}{\epsilon^2}}}{Z_\epsilon},$$

the constant Z_ϵ chosen so that $\int_{\mathbb{R}^m} \sigma^\epsilon \, d\xi = 1$. We once again write

$$u^\epsilon := \frac{\rho^\epsilon}{\sigma^\epsilon};$$

so that (3.2) becomes

$$\begin{cases} \tau_\epsilon \sigma^\epsilon (u^\epsilon_t - a\Delta_x u^\epsilon) = \operatorname{div}_\xi(\sigma^\epsilon D_\xi u^\epsilon) & \text{in } U \times \mathbb{R}^m \times [0,T] \\ \frac{\partial u^\epsilon}{\partial \nu} = 0 & \text{on } \partial U \times \mathbb{R}^m \times [0,T] \\ u^\epsilon = u^\epsilon_0 & \text{on } U \times \mathbb{R}^m \times \{t=0\}. \end{cases} \tag{3.4}$$

3.2 Estimates and convergence. We suppose that

$$0 \le u^\epsilon_0 \le C$$

and that

$$\int_{\mathbb{R}^m} \int_U (|u^\epsilon_0|^2 + |D_x u^\epsilon_0|^2 + \tfrac{1}{\tau_\epsilon} |D_\xi u^\epsilon_0|^2) \sigma^\epsilon \, dx d\xi < \infty. \tag{3.5}$$

Write

$$\mathbb{R}^m_\pm := \{\xi \in \mathbb{R}^m \mid \pm \xi_1 \ge 0\},$$

and also assume that as $\epsilon \to 0$

$$\begin{cases} u^\epsilon_0 \to 2\alpha_0 & \text{locally uniformly in } \bar{U} \times \mathbb{R}^m_- \\ u^\epsilon_0 \to 2\beta_0 & \text{locally uniformly in } \bar{U} \times \mathbb{R}^m_+, \end{cases} \tag{3.6}$$

where $\alpha_0 = \alpha_0(x)$ and $\beta_0 = \beta_0(x)$ are smooth.

Lemma 3.1. *We have the estimates*

$$0 \leq u^\epsilon \leq C$$

and

$$\sup_{0\leq t\leq T} \int_{\mathbb{R}^m} \int_U (|u^\epsilon|^2 + |D_x u^\epsilon|^2 + \tfrac{1}{\tau_\epsilon} |D_\xi u^\epsilon|^2) \sigma^\epsilon \, dx d\xi + \int_0^T \int_{\mathbb{R}^m} \int_U |u_t^\epsilon|^2 \, \sigma^\epsilon \, dx \, d\xi dt \leq C. \quad (3.7)$$

We again put $\gamma = \gamma(\epsilon) = \epsilon^{\frac{3}{4}}$; and for this higher-dimensional setting, define

$$I_\gamma := B(e^-, \gamma) \cup B(e^+, \gamma).$$

We will additionally write

$$B^\pm := B(e^\pm, r), \quad B := B^+ \cup B^-,$$

the radius $r > 0$ selected so small that $B^\pm \subset \{\Phi(\xi) \leq \frac{1}{4}\}$.

Lemma 3.2. *We have*

$$\int_{\mathbb{R}^m - I_\gamma} \sigma^\epsilon \, d\xi \to 0, \ \int_{B(e^\pm,\gamma)} \sigma^\epsilon \, d\xi \to \frac{1}{2}, \quad (3.8)$$

and

$$\int_{\{\Phi\geq 2\}} \frac{\sigma^\epsilon}{\tau_\epsilon} \, d\xi \to 0, \quad (3.9)$$

Lemma 3.3. (i) *There exists a subsequence $\epsilon = \epsilon_k \to 0$ and functions $\alpha, \beta \in H^1(U_T)$ such that*

$$\int_{B^-} \rho^\epsilon \, d\xi \rightharpoonup \alpha, \ \int_{B^+} \rho^\epsilon \, d\xi \rightharpoonup \beta \quad (3.10)$$

weakly in $L^2(U_T)$, and

$$\sup_{0\leq t\leq T} \int_{\mathbb{R}^m - B} |\rho^\epsilon| \, d\xi \to 0. \quad (3.11)$$

(ii) *In addition,*

$$\int_{B^-} \rho_t^\epsilon \, d\xi \rightharpoonup \alpha_t, \ \int_{B^+} \rho_t^\epsilon \, d\xi \rightharpoonup \beta_t \tag{3.12}$$

and

$$\int_{B^-} D_x\rho^\epsilon \, d\xi \rightharpoonup D_x\alpha, \ \int_{B^+} D_x\rho^\epsilon \, d\xi \rightharpoonup D_x\beta \tag{3.13}$$

weakly in $L^2(U_T)$*, with*

$$\int_{\mathbb{R}^m - B} \int_U |\rho_t^\epsilon| \, dx \, d\xi \to 0 \tag{3.14}$$

strongly in $L^2(0,T)$ *and*

$$\sup_{0 \le t \le T} \int_{\mathbb{R}^m - B} \int_U |D_x\rho^\epsilon| \, dx \, d\xi \to 0. \tag{3.15}$$

(iii) *For each time* $0 \le t \le T$ *and almost every* $x \in U$*, we have*

$$\begin{cases} u^\epsilon \to 2\alpha & \textit{for almost every } \ \xi \in B^- \\ u^\epsilon \to 2\beta & \textit{for almost every } \ \xi \in B^+ \end{cases} \tag{3.16}$$

as $\epsilon \to 0$.

3.3 Asymptotics and capacity estimates. We next recall Laplace's asymptotics in higher dimensions.

Lemma 3.4. *If* $f = f(\xi)$ *is a smooth function on* $\mathbb{R}^m$*, if* ξ_0 *is the unique maximum point of* f *and if* $D^2 f(\xi_0) < 0$*, then*

$$\int_{\mathbb{R}^m} e^{\frac{f(\xi)}{\epsilon^2}} \, d\xi = e^{\frac{f(\xi_0)}{\epsilon^2}} \frac{(2\pi\epsilon^2)^{\frac{m}{2}}}{\sqrt{|\det D^2 f(\xi_0)|}} (1 + o(1)) \qquad \textit{as } \epsilon \to 0. \tag{3.17}$$

We next follow Bovier–Eckhoff–Gayrard–Klein [B-E-G-K] and define the relative ϵ-*capacity* of the sets B^- and B^+ to be

$$\mathrm{Cap}_\epsilon(B^-, B^+) := \inf \left\{ \frac{1}{2} \int_{\mathbb{R}^m} e^{-\frac{\Phi}{\epsilon^2}} |D\psi|^2 \, d\xi \ \mid \ \psi|_{B^-} = -1, \psi|_{B^+} = 1 \right\}, \tag{3.18}$$

the infimum taken over C^1 functions $\psi : \mathbb{R}^m \to \mathbb{R}$.

Lemma 3.5. *As $\epsilon \to 0$, we have*

$$Z_\epsilon = \frac{2(2\pi\epsilon^2)^{\frac{m}{2}}}{\sqrt{|\det D^2\Phi(e^\pm)|}}(1+o(1)) \tag{3.19}$$

and

$$\mathrm{Cap}_\epsilon(B^-, B^+) = 2e^{-\frac{1}{\epsilon^2}}(2\pi\epsilon^2)^{\frac{m-2}{2}} \frac{|\lambda_1(0)|}{\sqrt{|\det D^2\Phi(0)|}}(1+o(1)). \tag{3.20}$$

Proof. Since there are two wells of equal depth at $e^\pm$ and since $\Phi(e^\pm) = 0$, Lemma 3.4 implies (3.19). The assertion (3.20) is due to [B-E-G-K], whose statement differs somewhat as we are using ϵ^2 in place of their ϵ and have normalized differently in the definition of capacity.

□

The primary technical problem we confront is identifying in higher dimensions a good analog of the function $\phi^\epsilon = \phi^\epsilon(\xi)$ used in the proof of Theorem 2.5.

Lemma 3.6. (i) *For each $\epsilon > 0$, there exists a function $\phi^\epsilon = \phi^\epsilon(\xi)$ belonging to $W^{2,p}_{loc}(\mathbb{R}^m)$ for all $1 \le p < \infty$ and solving the PDE*

$$-\operatorname{div}\left(\frac{\sigma^\epsilon}{\tau_\epsilon} D\phi^\epsilon\right) = \frac{1}{|B^+|}\chi_{B^+} - \frac{1}{|B^-|}\chi_{B^-}. \tag{3.21}$$

(ii) *In addition,*

$$\sup_{\mathbb{R}^m} |\phi^\epsilon| \le C, \tag{3.22}$$

for a constant independent of ϵ; and

$$\phi^\epsilon \to \begin{cases} \frac{1}{\kappa} & \text{uniformly on } B^+ \\ -\frac{1}{\kappa} & \text{uniformly on } B^-, \end{cases} \tag{3.23}$$

κ given by (3.1).

Above and in our subsequent discussion, we write $D\phi^\epsilon = D_\xi\phi^\epsilon$, $\Delta\phi^\epsilon = \Delta_\xi\phi^\epsilon$, etc.

Proof. 1. Define $\phi^\epsilon = \phi^\epsilon(\xi)$ to be a minimizer of

$$\frac{1}{2}\int_{\mathbb{R}^m} \frac{\sigma^\epsilon}{\tau_\epsilon}|D\phi|^2\,d\xi - \fint_{B^+}\phi\,d\xi + \fint_{B^-}\phi\,d\xi, \tag{3.24}$$

among all H^1_{loc} functions that are odd in the variable ξ_1. The slash through the integral signs means the average. The corresponding Euler–Lagrange equation is (3.21), and standard regularity theory implies $\phi^\epsilon \in W^{2,p}_{\text{loc}}$ for each $1 \leq p < \infty$.

We also have

$$\phi^\epsilon \geq 0 \quad \text{in } \mathbb{R}^m_+, \quad \phi^\epsilon \leq 0 \quad \text{in } \mathbb{R}^m_-,$$

as we could otherwise lower the energy by taking the odd function $\phi = (\phi^\epsilon)_+$ in $\mathbb{R}^m_+$ and $\phi = -(\phi^\epsilon)_-$ in $\mathbb{R}^m_-$. Define

$$\lambda_\epsilon := \fint_{B^+}\phi^\epsilon\,d\xi, \ \ \mu_\epsilon := \sup_{B^+}\phi^\epsilon.$$

Then $0 \leq \lambda_\epsilon \leq \mu_\epsilon$ and

$$\sup_{\mathbb{R}^m}|\phi^\epsilon| = \mu_\epsilon, \tag{3.25}$$

since otherwise $\phi = \Lambda(\phi^\epsilon)$ would give a smaller value in (3.24), where $\Lambda(s) = s$ if $-\mu_\epsilon < s < \mu_\epsilon$ and $\Lambda(s) = \pm\mu_\epsilon$ if $\pm s \geq \mu_\epsilon$.

2. Comparing with $\phi \equiv 0$ for the energy (3.24) gives the bound

$$\int_{\mathbb{R}^m} \frac{\sigma^\epsilon}{\tau_\epsilon}|D\phi^\epsilon|^2\,d\xi \leq 4\lambda_\epsilon. \tag{3.26}$$

We next use $\zeta\phi^\epsilon$ as a test function in the weak form of the Euler–Lagrange PDE, where the smooth, compactly supported function $\zeta = \zeta^R$ is identically 1 on the ball $B(R) = B(0,R)$ and satisfies $|D\zeta| \leq 1$. Then for large R we have

$$\int_{\mathbb{R}^m} \frac{\sigma^\epsilon}{\tau_\epsilon}|D\phi^\epsilon|^2\zeta\,d\xi = 2\lambda_\epsilon - \int_{\mathbb{R}^m} \frac{\sigma^\epsilon}{\tau_\epsilon}\phi^\epsilon D\phi^\epsilon \cdot D\zeta\,d\xi.$$

Now

$$\left|\int_{\mathbb{R}^m} \frac{\sigma^\epsilon}{\tau_\epsilon}\phi^\epsilon D\phi^\epsilon \cdot D\zeta\,d\xi\right| \leq \mu_\epsilon\left(\int_{\mathbb{R}^m} \frac{\sigma^\epsilon}{\tau_\epsilon}|D\phi^\epsilon|^2 d\xi\right)^{\frac{1}{2}}\left(\int_{\mathbb{R}^m - B(R)} \frac{\sigma^\epsilon}{\tau_\epsilon}\,d\xi\right)^{\frac{1}{2}}.$$

Using (3.26), we deduce upon sending $R \to \infty$ that

$$\int_{\mathbb{R}^m} \frac{\sigma^\epsilon}{\tau_\epsilon} |D\phi^\epsilon|^2 \, d\xi = 2\lambda_\epsilon. \tag{3.27}$$

3. Introduce the regions

$$\tilde{B}^\pm := B(e^\pm, 2r) \supset\supset B^\pm;$$

we may assume that r is small enough that $\tilde{B}^\pm \subset \{\xi \in \mathbb{R}^m \mid \Phi(\xi) \leq \frac{1}{3}\}$.

Then (3.27) and Poincare's inequality imply

$$\int_{\tilde{B}^+} |\phi^\epsilon - \tilde{\lambda}_\epsilon|^2 \, d\xi \leq C \int_{\tilde{B}^+} |D\phi^\epsilon|^2 \, d\xi \leq \frac{C}{\epsilon^2} e^{-\frac{2}{3\epsilon^2}} \lambda_\epsilon \leq C e^{-\frac{1}{2\epsilon^2}} \lambda_\epsilon \tag{3.28}$$

for

$$\tilde{\lambda}_\epsilon := \fint_{\tilde{B}^+} \phi^\epsilon \, d\xi.$$

We also compute

$$\begin{aligned} |\lambda_\epsilon - \tilde{\lambda}_\epsilon| &= \left| \fint_{B^+} \phi^\epsilon \, d\xi - \tilde{\lambda}_\epsilon \right| \leq \fint_{B^+} |\phi^\epsilon - \tilde{\lambda}_\epsilon| \, d\xi \\ &\leq C \int_{\tilde{B}^+} |\phi^\epsilon - \tilde{\lambda}_\epsilon| \, d\xi \leq C \left(\int_{\tilde{B}^+} |\phi^\epsilon - \tilde{\lambda}_\epsilon|^2 \, d\xi \right)^{\frac{1}{2}}. \end{aligned}$$

Therefore (3.28) implies

$$|\lambda_\epsilon - \tilde{\lambda}_\epsilon| \leq o(1) \lambda_\epsilon^{\frac{1}{2}}. \tag{3.29}$$

4. In $\mathbb{R}^m_+$, the PDE (3.21) reads

$$-\operatorname{div}\left(\frac{\sigma^\epsilon}{\tau_\epsilon} D\phi^\epsilon \right) = \frac{1}{|B^+|} \chi_{B^+}.$$

We expand the left hand side and recall the definition of σ^ϵ, to discover that

$$\begin{aligned} -\Delta(\phi^\epsilon - \tilde{\lambda}_\epsilon) &= -\frac{D\Phi \cdot D\phi^\epsilon}{\epsilon^2} + \frac{\tau_\epsilon}{\sigma^\epsilon} \frac{1}{|B^+|} \chi_{B^+} \\ &= -\frac{1}{\epsilon^2} \operatorname{div}((\phi^\epsilon - \tilde{\lambda}_\epsilon) D\Phi) + \frac{1}{\epsilon^2} \Delta\Phi (\phi^\epsilon - \tilde{\lambda}_\epsilon) + \frac{\tau_\epsilon}{\sigma^\epsilon} \frac{1}{|B^+|} \chi_{B^+}. \end{aligned} \tag{3.30}$$

Then interior elliptic estimates (see for instance Gilbarg–Trudinger [G-T, Theorem 8.17]) imply for any fixed $m < p < \infty$ that

$$||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^\infty(B^+)} \leq C||\tfrac{\tau_\epsilon}{\sigma^\epsilon}||_{L^\infty(B^+)} + \frac{C}{\epsilon^2}||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^p(\tilde{B}^+)} + C||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^2(\tilde{B}^+)}.$$

We may in particular assume $p > 2$. Therefore (3.25) and (3.28) let us calculate that as $\epsilon \to 0$

$$\begin{aligned} ||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^\infty(B^+)} &\leq o(1) + \frac{C}{\epsilon^2}||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^p(\tilde{B}^+)} + o(1)\lambda_\epsilon^{\frac{1}{2}} \\ &\leq o(1) + \frac{C}{\epsilon^2}||\phi^\epsilon - \tilde{\lambda}_\epsilon||^{1-\frac{2}{p}}_{L^\infty(\tilde{B}^+)}||\phi^\epsilon - \tilde{\lambda}_\epsilon||^{\frac{2}{p}}_{L^2(\tilde{B}^+)} + o(1)\lambda_\epsilon^{\frac{1}{2}} \\ &\leq o(1) + C||\phi^\epsilon - \tilde{\lambda}_\epsilon||^{1-\frac{2}{p}}_{L^\infty(\tilde{B}^+)}\lambda_\epsilon^{\frac{1}{p}}\frac{e^{-\frac{1}{2p\epsilon^2}}}{\epsilon^2} + o(1)\lambda_\epsilon^{\frac{1}{2}} \\ &\leq o(1)\left(1 + \lambda_\epsilon^{\frac{1}{2}} + ||\phi^\epsilon - \tilde{\lambda}_\epsilon||^{1-\frac{2}{p}}_{L^\infty(\tilde{B}^+)}\lambda_\epsilon^{\frac{1}{p}}\right). \end{aligned} \tag{3.31}$$

We have

$$||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^\infty(\tilde{B}^+)} \leq 2\mu_\epsilon = 2|\mu_\epsilon - \tilde{\lambda}_\epsilon| + 2\tilde{\lambda}_\epsilon.$$

As ϕ_ϵ attains its maximum μ_ϵ over $\mathbb{R}^m_+$ in B^+, we see also that

$$|\mu_\epsilon - \tilde{\lambda}_\epsilon| \leq ||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^\infty(B^+)}.$$

Hence (3.31) gives

$$||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^\infty(B^+)} \leq o(1)\left(1 + ||\phi^\epsilon - \tilde{\lambda}_\epsilon||^{1-\frac{2}{p}}_{L^\infty(B^+)}\lambda_\epsilon^{\frac{1}{p}} + \lambda_\epsilon^{1-\frac{1}{p}}\right). \tag{3.32}$$

It follows that

$$||\phi^\epsilon - \tilde{\lambda}_\epsilon||_{L^\infty(B^+)} \leq o(1)\left(1 + \lambda_\epsilon^{\frac{1}{2}} + \lambda_\epsilon^{1-\frac{1}{p}}\right) \leq o(1)\left(1 + \lambda_\epsilon^{1-\frac{1}{p}}\right).$$

Then (3.29) gives

$$||\phi^\epsilon - \lambda_\epsilon||_{L^\infty(B^+)} \leq o(1)\left(1 + \lambda_\epsilon^{1-\frac{1}{p}}\right). \tag{3.33}$$

It follows similarly that

$$||\phi^\epsilon + \lambda_\epsilon||_{L^\infty(B^-)} \leq o(1)\left(1 + \lambda_\epsilon^{1-\frac{1}{p}}\right). \tag{3.34}$$

5. We assert finally that

$$\lambda_\epsilon = \frac{1}{\kappa} + o(1). \tag{3.35}$$

This and (3.33), (3.34) will complete the proof.

Now according to (3.19), (3.20) and the definition of κ, we have

$$\inf\left\{\frac{1}{2}\int_{\mathbb{R}^m}\frac{\sigma^\epsilon}{\tau_\epsilon}|D\psi|^2\,d\xi \;\mid\; \psi|_{B^-}=-1, \psi|_{B^+}=1\right\} = \kappa + o(1). \tag{3.36}$$

Let ψ^ϵ denote a minimizer that is odd in the variable ξ_1. Then using $\phi = \lambda\psi^\epsilon$ as a competitor in (3.24) and recalling (3.27), we estimate

$$\begin{aligned} -\lambda_\epsilon &= \frac{1}{2}\int_{\mathbb{R}^m}\frac{\sigma^\epsilon}{\tau_\epsilon}|D\phi^\epsilon|^2\,d\xi - 2\lambda_\epsilon \\ &\le \frac{\lambda^2}{2}\int_{\mathbb{R}^m}\frac{\sigma^\epsilon}{\tau_\epsilon}|D\psi^\epsilon|^2\,d\xi - 2\lambda \\ &= \lambda^2\kappa - 2\lambda + o(1). \end{aligned}$$

Minimizing over λ, we see that $-\lambda_\epsilon \le -\frac{1}{\kappa} + o(1)$; thus $\frac{1}{\kappa} \le \liminf_{\epsilon\to 0}\lambda_\epsilon$. In particular, λ_ϵ is bounded away from 0.

Next note from (3.33) and (3.34) that $\frac{\phi^\epsilon}{\lambda_\epsilon} \to \pm 1$ uniformly on $B^\pm$. (This assertion is valid even if $\lambda_\epsilon \to \infty$, a possibility we have not yet eliminated.) Fix a small number $\delta > 0$ and define

$$\psi := \frac{1}{1-\delta}\Lambda\left(\tfrac{\phi^\epsilon}{\lambda_\epsilon}\right),$$

where now $\Lambda(s) = s$ if $-1+\delta < s < 1-\delta$ and $\Lambda(s) = \pm(1-\delta)$ if $\pm s \ge 1-\delta$. Observe that for small enough ϵ, we have $\psi \equiv \pm 1$ on $B^\pm$. Our employing ψ as a competitor in (3.36) gives

$$\begin{aligned} \kappa + o(1) &\le \frac{1}{2}\int_{\mathbb{R}^m}\frac{\sigma^\epsilon}{\tau_\epsilon}|D\psi|^2\,d\xi \\ &= \frac{1}{2(1-\delta)^2\lambda_\epsilon^2}\int_{\mathbb{R}^m}\frac{\sigma^\epsilon}{\tau_\epsilon}|D\phi^\epsilon|^2(\Lambda')^2\,d\xi \\ &\le \frac{1}{2(1-\delta)^2\lambda_\epsilon^2}\int_{\mathbb{R}^m}\frac{\sigma^\epsilon}{\tau_\epsilon}|D\phi^\epsilon|^2\,d\xi \\ &= \frac{1}{2(1-\delta)^2\lambda_\epsilon^2}2\lambda_\epsilon. \end{aligned}$$

Hence

$$\lambda_\epsilon \le \frac{1}{(1-\delta)^2\kappa} + o(1).$$

This inequality is valid for each $\delta > 0$ provided ϵ is small enough; consequently, $\limsup_{\epsilon\to 0} \lambda_\epsilon \le \frac{1}{\kappa}$. $\square$

3.4 Derivation of the reaction-diffusion system.

Theorem 3.7. *For all* $0 \le t \le T$*, we have*

$$\rho^\epsilon \rightharpoonup \alpha\delta_{e^-} + \beta\delta_{e^+}, \tag{3.37}$$

where the smooth functions $\alpha = \alpha(x,t)$ *and* $\beta = \beta(x,t)$ *solve the linear reaction-diffusion system*

$$\begin{cases} \alpha_t - a^-\Delta\alpha = \kappa(\beta-\alpha) & \text{in } U_T \\ \beta_t - a^+\Delta\beta = \kappa(\alpha-\beta) & \text{in } U_T \\ \frac{\partial\alpha}{\partial\nu} = \frac{\partial\beta}{\partial\nu} = 0 & \text{on } \partial U \times [0,T] \\ \alpha = \alpha_0, \beta = \beta_0 & \text{on } U \times \{t=0\}, \end{cases} \tag{3.38}$$

for $a^\pm := a(e^\pm)$.

Proof. 1. Select $\zeta \in C^\infty(U_T)$, $\zeta = \zeta(x,t)$; and let $\psi = \psi(\xi)$ be a smooth function supported on $\{\Phi \le 3\}$ such that $\psi \equiv 1$ on $\{\Phi \le 2\}$.

Multiplying (3.4) by $\psi\phi^\epsilon\zeta$ and integrating by parts, we get

$$\int_0^T\int_U\int_{\{\Phi\le 3\}} \psi\phi^\epsilon\zeta u_t^\epsilon\sigma^\epsilon\, d\xi dx dt + \int_0^T\int_U\int_{\{\Phi\le 3\}} \psi\phi^\epsilon a^\epsilon D_x u^\epsilon\cdot D_x\zeta\sigma^\epsilon\, d\xi dx dt$$
$$= -\int_0^T\int_U\int_{\{\Phi\le 3\}} \zeta\frac{\sigma^\epsilon}{\tau_\epsilon} D_\xi(\psi\phi^\epsilon)\cdot D_\xi u^\epsilon\, d\xi dx dt. \tag{3.39}$$

2. We then write $u_t^\epsilon\sigma^\epsilon = \rho_t^\epsilon$ and argue as in the previous proof, using (3.23) to find

$$\lim_{\epsilon\to 0}\int_0^T\int_U\int_{\{\Phi\le 3\}} \psi\phi^\epsilon\zeta u_t^\epsilon\sigma^\epsilon\, d\xi dx dt = \frac{1}{\kappa}\int_0^T\int_U (\beta_t-\alpha_t)\zeta\, dx dt \tag{3.40}$$

and

$$\lim_{\epsilon\to 0}\int_0^T\int_U\int_{\{\Phi\le 3\}}\psi\phi^\epsilon a^\epsilon D_x u^\epsilon\cdot D_x\zeta\sigma^\epsilon\,d\xi dxdt$$
$$=\frac{1}{\kappa}\int_0^T\int_U(a^+D_x\beta-a^-D_x\alpha)\cdot D_x\zeta\,dxdt. \quad (3.41)$$

3. We write out the last term in (3.39) as

$$\int_0^T\int_U\int_{\{\Phi\le 3\}}\psi\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}D\phi^\epsilon\cdot D_\xi u^\epsilon\,d\xi dxdt+\int_0^T\int_U\int_{\{\Phi\le 3\}}\phi^\epsilon\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}D\psi\cdot D_\xi u^\epsilon d\xi dxdt$$
$$=-\int_0^T\int_U\int_{\{\Phi\le 3\}}\psi\zeta\mathrm{div}\left(\frac{\sigma^\epsilon}{\tau_\epsilon}D\phi^\epsilon\right)u^\epsilon\,d\xi dxdt$$
$$-\int_0^T\int_U\int_{\{\Phi\le 3\}}u^\epsilon\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}D\psi\cdot D\phi^\epsilon\,d\xi dxdt+\int_0^T\int_U\int_{\{\Phi\le 3\}}\phi^\epsilon\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}D\psi\cdot D_\xi u^\epsilon d\xi dxdt.$$

Since $D\psi\equiv 0$ on $\{\Phi\le 2\}$, second and third terms are estimated by

$$C\left(\int_0^T\int_U\int_{\mathbb{R}^m}(|D_\xi u^\epsilon|^2+|D\phi^\epsilon|^2)\frac{\sigma^\epsilon}{\tau_\epsilon}d\xi dxdt\right)^{\frac12}\left(\int_{\{2\le\Phi\le 3\}}\frac{\sigma^\epsilon}{\tau_\epsilon}\,d\xi\right)^{\frac12}\to 0,$$

according to (3.9). Furthermore, the PDE (3.21) implies

$$-\int_0^T\int_U\int_{\{\Phi\le 3\}}\psi\zeta\mathrm{div}\left(\frac{\sigma^\epsilon}{\tau_\epsilon}D\phi^\epsilon\right)u^\epsilon\,d\xi dxdt$$
$$=\int_0^T\int_U\zeta\left(⨍_{B^+}u^\epsilon\,d\xi-⨍_{B^-}u^\epsilon\,d\xi\right)dxdt$$

Hence (3.23) gives

$$\lim_{\epsilon\to 0}\int_0^T\int_U\int_{\{\Phi\le 3\}}\zeta\frac{\sigma^\epsilon}{\tau_\epsilon}D_\xi(\psi\phi^\epsilon)\cdot D_\xi u^\epsilon\,d\xi dxdt=2\int_0^T\int_U\zeta(\beta-\alpha)\,dxdt. \quad (3.42)$$

4. Sending $\epsilon\to 0$, we conclude from (2.29) and (2.30)–(2.32) that α,β satisfy the integral identity

$$\int_0^T\int_U(\beta_t-\alpha_t)\zeta\,dxdt+\int_0^T\int_U(a^+D_x\beta-a^-D_x\alpha)\cdot D_x\zeta\,dxdt$$
$$=-2\kappa\int_0^T\int_U(\beta-\alpha)\zeta\,dxdt$$

for all test functions ζ. Consequently,

$$\beta_t - \alpha_t - (a^+\Delta\beta - a^-\Delta\alpha) = 2\kappa(\alpha - \beta).$$

As in the previous section, we also have

$$\beta_t + \alpha_t - (a^+\Delta\beta + a^-\Delta\alpha) = 0;$$

the PDE in (3.38) for α and β follow. □

References

[A-M-P-S-V] S. Arnrich, A. Mielke, M. A. Peletier, G. Savare, M. Veneroni, Passage to the limit in a Wasserstein gradient flow: from diffusion to reaction, Calculus of Variations and Partial Differential Equations, 44 (2012), 419–454.

[B] N. Berglund, Kramers' law: validity, derivations and generalisations, Markov Process Related Fields 19 (2013), 459–490.

[B-O] C. Bender and S. Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, 1978.

[B-E-G-K] A. Bovier, M. Eckhoff, V. Gayrard and M. Klein, Metastability in reversible diffusion processes. I. Sharp asymptotics for capacities and exit times, J. Eur. Math. Soc. 6 (2004), 399–424.

[G-T] D. Gilbarg and N. Trudinger, *Elliptic Partial Differential Equations of Second Order*, 2nd ed, Springer, 1983.

[H-N] M. Herrmann and B. Niethammer, Kramers' formula for chemical reactions in the context of Wasserstein gradient flows, Comm Math Sci 9 (2011), 623–635.

[L] G. Lieberman, *Second Order Parabolic Differential Equations*, World Scientitic Publishing, 1996.

[P-S-V1] M. A. Peletier, G. Savare and M. Veneroni, From diffusion to reaction via Γ-convergence, SIAM J. Math. Analysis 42 (2010), 1805–1825.

[P-S-V2] M. A. Peletier, G. Savare and M. Veneroni, Chemical reactions as Γ-limit of diffusion, SIAM Review 54 (2012), 327–352.