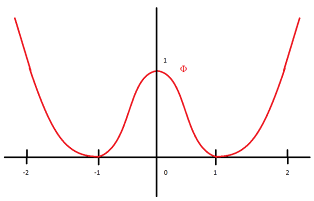
1 Past research

1.1 The Kramers-Smoluchowski equation

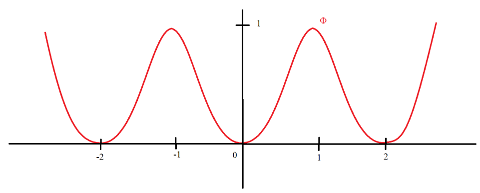
Introduction My research interests lie primarily in the field of partial differential equations (PDE) and the calculus of variations. I am interested in studying various asymptotic limits that arise in PDE, such as in chemical reactions. More precisely, consider the following one-dimensional **Kramers-Smoluchowski equation:**

$$\tau_\epsilon \left(\rho^\epsilon_t - a\Delta_x \rho^\epsilon\right) = \left(\rho^\epsilon_\xi + \epsilon^{-2}\rho^\epsilon \Phi'(\xi)\right)_\xi \tag{KS$_\epsilon$}$$

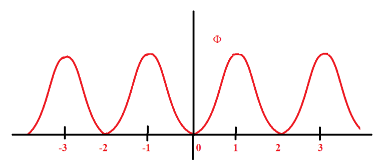
Here $\rho^\epsilon = \rho^\epsilon(x,\xi,t) : U \times \mathbb{R} \times [0,T] \to \mathbb{R}$ (U open and bounded in $\mathbb{R}^n$), $\tau_\epsilon = \frac{1}{\epsilon^2} e^{-\frac{1}{\epsilon^2}}$, $a = a(\xi)$ is bounded and positive, $\Phi : \mathbb{R} \to \mathbb{R}$, $\Phi = \Phi(\xi)$ is an even double-well potential function as depicted in Figure (a), normalized so that $\Phi(0) = 1, \Phi(\pm 1) = 0, \Phi(\pm 2) = 1$:



(a) Double-Well Potential



(b) Triple-Well Potential



(c) Infinitely many Wells

By defining $\sigma^\epsilon = \frac{e^{-\frac{\Phi}{\epsilon^2}}}{Z_\epsilon}$, where Z_ϵ makes $\int_{\mathbb{R}} \sigma^\epsilon = 1$, and letting $u^\epsilon =: \frac{\rho^\epsilon}{\sigma^\epsilon}$, we can normalize (KS$_\epsilon$) to become:

$$\tau_\epsilon \sigma^\epsilon \left(u^\epsilon_t - a^\epsilon \Delta_x u^\epsilon\right) = \left(\sigma^\epsilon u^\epsilon_\xi\right)_\xi \tag{KS$'_\epsilon$}$$

Chemical Context There are two different ways of viewing a chemical reaction. Consider a simple $A \rightleftharpoons B$-system, where a particle A reacts to become B, and vice-versa. On the other hand, the dynamics of the reaction are given by the classical reaction-diffusion system (R$-$D) (see below), where α is the density of A and β is the density of B. On the other hand, one can augment the system by adding a 'chemical' variable ξ, so that a chemical reaction corresponds to the movement of a particle from one local minimum (here $\xi = -1$, corresponding to A) to another ($\xi = 1$, corresponding to B). In that case, the dynamics of the reaction are given by an SDE, whose Fokker-Planck equation is (KS$_\epsilon$). The main result below shows that both points of view are just different sides of the same coin: one can take a limit of *large activation energy* $\frac{1}{\epsilon}$ of (KS$_\epsilon$) to obtain (R$-$D).

Main Result Using standard estimates, one can show that:

Theorem. *For all $0 \leq t \leq T$, we have:*

$$\rho^{\epsilon} \rightharpoonup \alpha\, \delta_{\{\xi=-1\}} + \beta\, \delta_{\{\xi=1\}}$$

where $\alpha = \alpha(x,t)$ and $\beta = \beta(x,t)$; and more importantly:

Theorem (Main Theorem)**.** *The functions α and β solve the following **linear reaction-diffusion system**, where $\kappa = \frac{\sqrt{|\Phi''(0)|\Phi''(1)}}{2\pi}$ and $d^{\pm} := a(\pm 1)$:*

$$\begin{cases} \alpha_t - d^{-}\Delta\alpha = \kappa(\beta - \alpha) \\ \beta_t - d^{+}\Delta\beta = \kappa(\alpha - \beta) \end{cases} \tag{R–D}$$

Idea of proof This result has already been proven by Peletier, Savaré, and Veneroni in [PSV12], using $\Gamma-$convergence. In [HN11], Herrmann and Niethammer provide a different proof, by rewriting (KS_{ϵ}) as a gradient flow on the Wasserstein space of probability measures and using a Rayleigh-type dissipation functional. In my thesis [Tab16] and in a joint paper with my advisor Lawrence C. Evans [ET16], we provide a direct proof that avoids the use of abstract machinery. The main idea is to devise a test function ϕ^{ϵ} which, after multiplying (KS_{ϵ}) by ϕ^{ϵ} and integrating by parts, cancels out the singular term σ^{ϵ} in ($KS_{\epsilon}^{'}$):

$$\phi^{\epsilon}(\xi) = \int_0^{\Lambda(\xi)} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \quad \text{where } \Lambda(s) = \begin{cases} -3/2 & \text{if} \quad s \leq -3/2 \\ s & \text{if} \quad -3/2 \leq s \leq 3/2 \\ 3/2 & \text{if} \quad s \geq 3/2 \end{cases}$$

The proof is robust enough that we can modify it to treat more general cases. All proofs rely on building test functions similar to ϕ^{ϵ} above.

1.2 Generalizations

Three wells: If Φ has three wells at $-2, 0, 2$ as in figure (b), then $\rho^{\epsilon} \rightharpoonup \alpha\, \delta_{-2} + \beta\, \delta_0 + \gamma\, \delta_2$, where α, β, δ solve (Here $d_i = a(i)$):

$$\begin{cases} \alpha_t - d_{-2}\, \Delta_x \alpha = \kappa\,(\beta - \alpha) \\ \beta_t - d_0\, \Delta_x \beta = \kappa\,(\alpha - 2\beta + \gamma) \\ \gamma_t - d_2\, \Delta_x \gamma = \kappa\,(\beta - \gamma) \end{cases} \tag{R-D}$$

Periodic wells: Take the triple-well case, but this time identify the points $-\frac{5}{2}$ and $\frac{7}{2}$ and modify σ^{ϵ} so that $\int_{-5/2}^{7/2} \sigma^{\epsilon} = 1$. Then we get the same result as for the triple-well-case.

Infinitely many wells: If $\Phi(2m) = 0$ for $m \in \mathbb{Z}$, as in Figure (c), then modifying Z_{ϵ} so that $\int_{-1}^{1} \sigma^{\epsilon} d\xi = 1$, we get that $\rho^{\epsilon} \rightharpoonup \sum_{m=-\infty}^{\infty} \alpha^m \delta_{2m}$ for functions α^m ($m \in \mathbb{Z}$), which satisfy the infinite system, where $d_{2m} =: a(2m)$:

$$\alpha_t^m - d_{2m}\Delta_x \alpha^m = 2\kappa\left(\alpha^{m-1} - 2\alpha^m + \alpha^{m+1}\right)$$

1.3 Higher-dimensional case

In the joint paper above [ET16], we were able to generalize this to the case where the chemical variable ξ is more than one-dimensional. Assume that $\Phi : \mathbb{R}^m \to \mathbb{R}$ is smooth, nonnegative, even in the first variable ξ_1, has two wells at the points $e^{\pm} = (\pm 1, 0, \cdots, 0)$, normalized so that $\Phi(0) = 1$, $\Phi(e^{\pm}) = 0$, and moreover $\det D^2\Phi(e^{\pm}) \neq 0$ and $D^2\Phi(0)$ is diagonal, with eigenvalues $\lambda_1(0) < 0 < \lambda_2(0) \leq \cdots \leq \lambda_m(0)$. Then the analog of $(\mathrm{KS}_\epsilon^{'})$ reads as:

$$\tau_\epsilon \sigma^\epsilon \left(u_t^\epsilon - a\Delta_x u^\epsilon\right) = \mathrm{div}_\xi \left(\sigma^\epsilon D_\xi u^\epsilon\right)$$

And we obtain that $\rho^\epsilon \rightharpoonup \alpha\delta_{e^-} + \beta\delta_{e^+}$, where α, β solve:

$$\begin{cases} \alpha_t - d^- \Delta_x \alpha = \kappa\left(\beta - \alpha\right) \\ \beta_t - d^+ \Delta_x \beta = \kappa\left(\alpha - \beta\right) \end{cases}$$

Here $d^{\pm} = a(e^{\pm})$ and $\kappa = \frac{|\lambda_1(0)|}{2\pi} \frac{\sqrt{|\det D^2\Phi(e^{\pm})|}}{\sqrt{|\det D^2\Phi(0)|}}$

In this case, to calculate κ, we use capacity-methods, and to construct our test-function ϕ^ϵ, we show that there exists a solution to the following PDE, where $B^{\pm} =: \left\{\Phi(\xi) \leq \frac{1}{4}\right\} \cap \mathbb{R}^m_{\pm}$:

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

2 Ongoing and Future Research Projects

2.1 Multidimensional Triple−Well Case

Equilateral Triangle: Take the multidimensional case above, but this time assume that there are three wells arranged in an equilateral triangle and connected by saddle points that are on the midpoints of each side. The trick here is to construct test functions that are solutions to PDE like above, with reflective symmetry properties. Currently, I'm working on the case where the triangle above is not equilateral, as well as figures where there's an uneven number of wells connected to each other, as for instance a kite (the convex hull of a cross). We could then ask ourselves "What if the wells are arranged in a *graph*, where any two vertices are connected by an edge going through one saddle point?" and perhaps connect this idea with graph theory, and there could potentially be applications of this to communication theory, where each well 'communicates' with another through a saddle point.

Revolution-well: Now take the one-dimensional well in the $yz-$plane, and rotate it around the $z-$axis to obtain a hat-like figure. One can then show that the solutions concentrate on the unit circle $x^2 + y^2 = 1$ in the $xy-$plane, but it is not clear what the resulting equations would look like.

Translation-well: This time, take the parabola $z = y^2$ in the $yz-$plane and just translate it along the $x-$axis. In that case, the solution concentrate along the x-axis but again it would be interesting to see what the resulting equation looks like.

2.2 Systems of (K-S) equations

Consider the system

$$\sigma^\epsilon \mathbf{u}^\epsilon_t - \sigma^\epsilon \Delta \mathbf{u}^\epsilon = \left(\frac{\sigma^\epsilon}{\tau_\epsilon} A \mathbf{u}^\epsilon_\xi \right)_\xi,$$

where $\mathbf{u}^\epsilon = (u^\epsilon_1, \cdots u^\epsilon_m)$ and A satisfies an ellipticity condition, then we get that $\sigma^\epsilon \mathbf{u}^\epsilon \rightharpoonup \boldsymbol{\alpha}\delta_{-1} + \boldsymbol{\beta}\delta_1$, where $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_m)$ and $\boldsymbol{\beta} = (\beta_1, \cdots, \beta_m)$ solve the system:

$$\begin{cases} \boldsymbol{\alpha}_t - \Delta \boldsymbol{\alpha} = \kappa A(\boldsymbol{\beta} - \boldsymbol{\alpha}) \\ \boldsymbol{\beta}_t - \Delta \boldsymbol{\beta} = \kappa A(\boldsymbol{\alpha} - \boldsymbol{\beta}) \end{cases}$$

It would be interesting to study the case where A is a nonlinear operator instead of a matrix.

2.3 The nonlinear case

Variant 1: Consider the nonlinear (KS$_\epsilon$)-equation, with f' bounded:

$$\sigma^\epsilon u^\epsilon_t - \sigma^\epsilon \Delta[f(u^\epsilon)] = \left(\frac{\sigma^\epsilon}{\tau_\epsilon} [f(u^\epsilon)]_\xi \right)_\xi,$$

Then the result is the same as usual (with a similar proof), except that here α and β solve

$$\begin{cases} \alpha_t - \operatorname{div}[f'(2\alpha)(\nabla\alpha)] = \frac{\kappa}{2}[f(2\beta) - f(2\alpha)] \\ \beta t - \operatorname{div}[f'(2\beta)(\nabla\beta)] = \frac{\kappa}{2}[f(2\alpha) - f(2\beta)] \end{cases}$$

Note that one can easily generalize this result to the case of systems as well.

Variant 2: A perhaps more interesting variant would be to study

$$\sigma^\epsilon u^\epsilon_t - \Delta u^\epsilon = \left(\frac{\sigma^\epsilon}{\tau_\epsilon} f(u^\epsilon_\xi) \right)_\xi,$$

In this case f satsifies a monotonicity condition $xf(x) \geq C|x|^2$ for some $C > 0$. Although the convergence results are the same, it is not clear at all what the resulting PDE looks like. In the linear case, we have a representation formula for u^ϵ:

$$u^\epsilon(x,\xi,t) = \kappa(\beta(x,t) - \alpha(x,t)) \left(\int_0^\xi \frac{\tau_\epsilon}{\sigma^\epsilon} d\xi \right) + (\alpha(x,t) + \beta(x,t)),$$

And I am currently trying to find one for the nonlinear case. Moreover, as suggested in [PSV12] in the linear case, perhaps the stationary solution of (K-S) is useful, which is here

$$u^\epsilon(x,\xi,t) = \int_0^\xi f^{-1} \left(A(x,t) \frac{\tau_\epsilon}{\sigma^\epsilon(\xi)} \right) d\xi + B(x,t)$$

2.4 Other nonlinear PDE I'm interested in exploring

A Fisher-KPP-system: In [BRR13], Berestycki, Roquejoffre, and Rossi study a system modeling the interaction between two biological populations, $u = u(x,t)$ on the road, and $v = v(x,y,t)$ in a field $(y \geq 0)$, where f satisfies a certain Fisher-KPP assumption.

$$\begin{cases} u_t - Du_{xx} = \nu v(x,0,t) - \mu u \\ v_t - dv_{xx} - dv_{yy} = f(v) \\ -dv_y(x,0,t) = \mu u - \nu v(x,0,t) \end{cases}$$

The authors show that there exists an *asymptotic speed of propagation* (ASP) $c_* > 0$, which is a certain bifurcation-value for the behavior of u and v. They study the values of c^* in terms of linear regions $|x| \leq ct$, but it would be interesting to see what happens when we study nonlinear regions, say $|x| \leq c\log(t)$. Also how does c^* depend on the parameters μ, ν, D, d?

A homogenization model for motor proteins: In [MS13] by Souganidis and Mirrahimi study the following Fokker-Planck equation which models the motion of motor proteins along a molecular filament, with ψ, ν, μ are positive and $1-$periodic:

$$\begin{cases} u_t^\epsilon - \epsilon\Delta_x u^\epsilon - \operatorname{div}_x \left(u^\epsilon D_y \psi \left(\frac{x}{\epsilon} \right) \right) = \frac{1}{\epsilon} \left(\nu \left(\frac{x}{\epsilon} \right) v^\epsilon - \mu \left(\frac{x}{\epsilon} \right) u^\epsilon \right) \\ v_t^\epsilon - \epsilon\Delta_x v^\epsilon = \frac{1}{\epsilon} \left(\mu \left(\frac{x}{\epsilon} \right) u^\epsilon - \nu \left(\frac{x}{\epsilon} \right) v^\epsilon \right) \end{cases}$$

In the linear case, the authors show that the proteins move along a fixed filament with a constant speed, that is

$$u^\epsilon(x,t) + v^\epsilon(x,t) \rightharpoonup \delta(x - \mathbf{v}t) I_0$$

for some $\mathbf{v} \in \mathbb{R}^d$ and $I_0 > 0$. I would like to explore what happens when we study the non-linear case, e.g. if the right-hand-side of both equations depend nonlinearly on $u^\epsilon, v^\epsilon, \mu, \nu$.

The G-equation Finally, inspired by the works of Jack Xin and Yifeng Yu [XY14], I would like to study the following $G-$equation, a Hamilton-Jacobi equation modeling turbulent combustion:

$$\begin{cases} G_t + AV(x) \cdot DG + |DG| = 0 \\ G(x,0) = p \cdot x, \end{cases}$$

for $V(x,y,z) = (C\cos(y) + A\sin(z), B\sin(x) + A\cos(z), B\cos(x) + C\sin(y))$. Numerical simulations show that the turbulent flame speed $s_T(p,A) =: \lim_{t\to\infty} \frac{-G(x,t)}{t}$ grows linearly with A as $A \to \infty$ (p is any unit vector in $\mathbb{R}^3$); I am proposing to prove this claim rigorously.

References

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