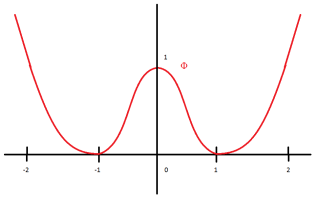
1 Past and current research

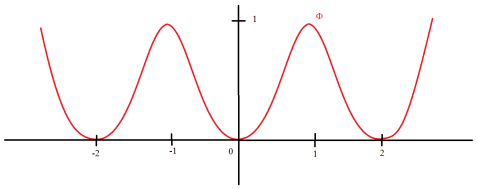
Introduction My research lies primarily in the field of partial differential equations (PDE) and the calculus of variations. I am interested in studying various asymptotic limits that arise in PDE, such as in chemical reactions. More precisely, consider the following one-dimensional **Kramers-Smoluchowski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

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

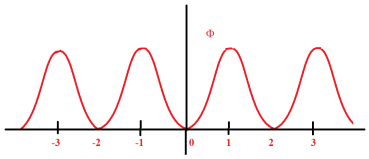
Here $\rho^\epsilon = \rho^\epsilon(x,\xi,t) : U \times \mathbb{R} \times [0,T] \to \mathbb{R}$ (U open and bounded in $\mathbb{R}^n$), $\tau_\epsilon = \frac{1}{\epsilon^2} e^{-\frac{1}{\epsilon^2}}$, $a = a(\xi)$ is bounded and positive, $\Phi : \mathbb{R} \to \mathbb{R}$, $\Phi = \Phi(\xi)$ is an 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:

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

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 ($\text{KS}_\epsilon^{'}$):

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

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.

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 $d_{2m} =: a(2m)$:

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

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 (KS'_ϵ) reads as:

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

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

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

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 $B^{\pm} =: \left\{\Phi(\xi) \leq \frac{1}{4}\right\} \cap \mathbb{R}^m_{\pm}$:

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

2 Future and Planned Research

In my postdoctoral studies, I intend to study more general asymptotic PDE models, including but not limited to chemical reactions. The following is a list of possible research topics that I am interested in.

Nonlinear Chemical Reactions and Diffusions One idea is to work on an extension of the chemical reactions and diffusions-paper: Since I am interested in nonlinear PDE, I ultimately would like to find an equation similar to (KS_ϵ) with the property that the solutions $\rho^\epsilon \rightharpoonup \alpha\delta_{-1} + \beta\delta_1$, but this time α and β solve a nonlinear reaction-diffusion system, where ψ^i are nonlinear functions of α, β:

$$\begin{cases} \alpha_t - d^-\Delta_x \alpha = \psi^1(\alpha, \beta) \\ \alpha_t - d^+\Delta_x \beta = \psi^2(\alpha, \beta) \end{cases}$$

One approach would be to work backwards in the direct proof I provided, and to see how, after cancellation with the test-function ϕ^ϵ, instead of getting $\int (u^\epsilon)_\xi$, one can obtain an expression of the form $\int (\psi(u^\epsilon))_\xi \, d\xi$ for some suitable nonlinear ψ.

A Fisher-KPP-system I am also interested in reaction-diffusions systems arising in Biology, in particular the works of Henri Berestycki. In their paper [BRR13], Berestycki, Roquejoffre, and Rossi study a system modeling the interaction between two populations, one $u = u(x,t)$ on a road and another one $v = v(x,y,t)$ in a field ($x \in \mathbb{R}, y \in \mathbb{R}^+$), where f is of Fisher-KPP-type, meaning that $f(0) = f(1) = 0$ and $0 < f(s) \leq f'(0)s$ on $(0,1)$:

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

The authors show that there is an *asymptotic speed of propagation* (ASP) $c_* = c_*(\mu, \nu, d, D) > 0$ for which:

- For all $c > c_*$, $\lim_{t\to\infty} \sup_{|x|\geq ct}(u(x,t), v(x,y,t)) = (0,0)$
- For all $c < c_*$, $\lim_{t\to\infty} \sup_{|x|\leq ct}(u(x,t), v(x,y,t)) = \left(\frac{\nu}{\mu}, 1\right)$

I would like to study to what extent the above result can be refined. What happens to u and v if we replace the region $\{(x,y) \in \mathbb{R} \times \mathbb{R}_{\geq 0}, |x| \leq ct\}$ by the region, say, $|x| \leq c\log(t)$? Would we get an even larger ASP there? Would the convergence be exponentially fast? It is also shown that if $D > 2d$, then $\widetilde{c}(\mu,\nu,d) =: \lim_{D\to\infty} \frac{c_*(\mu,\nu,d,D)}{\sqrt{D}}$ exists. How does $\widetilde{c}$ depend on the parameters μ, ν, d?

A homogenization model for motor proteins Staying within the realm of Biology, I am also interested in studying a nonlinear version of the following Fokker-Planck system analyzed in the paper [MS13] by Souganidis and Mirrahimi (where $\mu, \nu, \psi > 0$ are $1-$periodic), which models the motion of motor proteins along molecular filaments:

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

In the linear case, the authors show that the proteins move along a fixed filament with a constant speed $\mathbf{v} \in \mathbb{R}^d$, where $I_0 =: \lim_{\epsilon\to 0}\int_{\mathbb{R}^d} u^\epsilon(x,0) + v^\epsilon(x,0)dx$:

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

I would like to analyze to what extent this result still holds in the nonlinear case, where Φ and Ψ are suitable nonlinear functions of their arguments:

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

The G-equation Finally, inspired by the works of Jack Xin and Yifeng Yu on combustion theory [XY14], I would like to study the following $G-$equation, a Hamilton-Jacobi equation modeling turbulent combustion, in the case where $n = 3$ with $V(x, y, z) = (C\cos(y) + A\sin(z), B\sin(x) + A\cos(z), B\cos(x) + C\sin(y))$, the chaotic Arnold-Beltrami-Childress flow:

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

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.

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