# Reaction-Diffusion (-Convection) Equations, Entropies and Sobolev Inequalities

Peter A. Markowich

DAMTP, University of Cambridge

mainly based on joint work with M. Di Francesco, K. Fellner, H.Wu and S.Zheng

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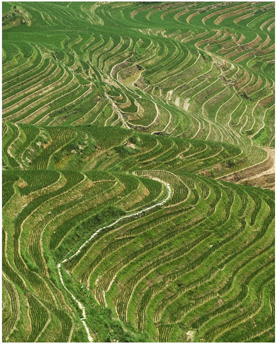
# Areas of Applications

Population dynamics: predator-prey systems

# Heterogeneous environments

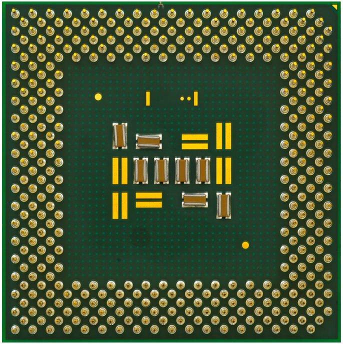
*"In the last two decades, it has become increasingly clear that the spatial dimension and, in particular, the interplay between environmental heterogeneity and individual movement, is an extremely important aspect of ecological dynamics." (P. Turchin)*



# Pattern formation: Turing instability

# Chemotaxis: Keller-Segel system

# Semiconductor modelling: drift-diffusion equations



# Mathematical Form of Reaction-Diffusion Equations

Particle ensembles undergo:

1. A Brownian motion leading to diffusion
2. Instantaneous reactions with each other and/or their environment
3. Convection by force fields, either external or self-consistent.

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$$u_t = -\operatorname{div} J(x,t) + \operatorname{div}(E_1(x,t)u, \ldots, E_m(x,t)u) + F(x,t,u)\ ,$$
$$x \in G\ ,\ \ t > 0$$

$$\text{Fick type law:} \quad J(x,t) = -D(x,t,u)\nabla u(x,t)$$

This parabolic system has to be supplemented by initial and boundary conditions.

# Main topic of this talk: Large-time Asymptotics

1. Do equilibria exist? Uniqueness?
2. Convergence of solutions as $t \to \infty$.
3. Rates of convergence! Exponential? Algebraic?
4. Optimal Rates!

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(Some) Issues:

- Nonlinearities
- Boundary conditions
- Turing instability

# Heat Equation: Dirichlet Problem

$$\begin{cases} u_t = \Delta u \ , \quad x \in G \text{ ...bounded domain in } \mathbb{R}^d \\ u\Big|_{\partial G} = 0 \\ u(t=0) = u_I \end{cases}$$

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unique equilibrium: $u \equiv 0$, no degree of freedom!

$$H_0^1(G) - \text{Poincaré inequality:} \quad \int u^2 \, dx \leq C_G^2 \int |\nabla u_I|^2 \, dx \ \forall \ u \in H_0^1(G)$$

$$\frac{1}{2} \frac{d}{dt} \int_G u^2 \, dx = - \int_G |\nabla u|^2 \, dx \leq - \frac{1}{C_G^2} \int_G u^2 \, dx$$
$$\Rightarrow \int_G u^2(x,t) \, dx \leq \exp\left( - \frac{2t}{C_G^2} \right) \int_G u^2 \, dx$$

$C_G$...Poincaré constant of $G$, sharp estimate, simple spectral theory, ...

# Heat Equation: Neumann Problem

$$\begin{cases} u_t = \Delta u \;, \quad x \in G \;, \quad t > 0 \\ \nabla u \cdot n \Big|_{\partial G} = 0 \;, \quad t > 0 \\ u(t=0) = u_I \end{cases}$$

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$H^1(G)$-Poincaré inequality:

$$\int_G (u - \bar{u})^2 \, dx \leq D_G^2 \int_G |\nabla u|^2 \, dx \,, \quad \forall u \in H^1(G) \,, \quad \bar{u} := \frac{1}{\mathrm{vol}(G)} \int_G u \, dx$$

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decay estimate: $$\int_G (u(x,t) - \bar{u}_I)^2 \, dx \leq \exp\left(-\frac{2t}{D_G^2}\right) \int_G (u_I - \bar{u}_I)^2 \, dx$$

# Neumann Problem with linear Reaction

$$\begin{cases} u_t = \Delta u - \lambda u \,, \quad x \in G \,, \quad t > 0 \,, \quad \lambda > 0 \\ \nabla u \cdot n \Big|_{\partial G} = 0 \,, \quad t > 0 \\ u(t = 0) = u_I \end{cases}$$

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but:

$$\int_G (u(x,t) - \bar{u}(t))^2 \, dx \le \exp\left(-2\left(\frac{1}{D_G^2} + \lambda\right) t\right) \int_G (u_I - \bar{u}_I)^2 \, dx$$

# Diffusion-Convection on $\mathbb{R}^d$: Entropies

Fokker-Planck equation: $$\begin{cases} u_t = \operatorname{div}\left(\nabla u + u\nabla A(x)\right) \;, \quad x \in \mathbb{R}^d \;, \quad t > 0 \\ u(t=0) = u_I \end{cases}$$

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Assumptions:

1. $A$ is $\omega$-convex: $D^2 A(x) \geq \omega \mathrm{I}$ on $\mathbb{R}^d$
2. w.l.o.g: $\int_{\mathbb{R}^d} e^{-A}\, dv = 1$
3. $u_I \in L^1(\mathbb{R}^d)$, $\int_{\mathbb{R}^d} u_I \, dx = 1$.

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equilibria: $u = \mathrm{const}.e^{-A(x)}$...one degree of freedom
mass conservation: expect $u(x,t) \to e^{-A(x)} =: u_\infty$ as $t \to \infty$.

$$u_t = \operatorname{div}\left(u_\infty \nabla\left(\frac{u}{u_\infty}\right)\right)$$

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Def: $\Phi'' \geq 0$, $\Phi''(s) \neq 0 \ \forall s$, $\Phi(1) = 0$, $\Phi'(1) = 0$, $(\Phi''')^2 \leq \frac{1}{2}\Phi''\Phi''''$.
Then $\Phi$ is called an admissible entropy generator.

note: $\int u \, dx = \int u_\infty \, dx$, $\Phi$ admissible $\Rightarrow e_\Phi(u|u_\infty) \geq 0$, $I_\Phi(u|u_\infty) \geq 0$ $(= 0 \text{ iff } u \equiv u_\infty)$

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Sobolev inequality:

$$\int_{\mathbb{R}^d} \Phi\left(\frac{u}{u_\infty}\right) \, du_\infty \leq \frac{1}{2\omega} \int_{\mathbb{R}^d} \Phi''\left(\frac{u}{u_\infty}\right) \left|\nabla\left(\frac{u}{u_\infty}\right)\right|^2 du_\infty ,$$

if $\Phi$ admissible, $\int u \, dx = \int u_\infty \, dx$, $u \geq 0$, $u_\infty \geq 0$, $u_\infty$ is $(-\omega)$-log-concave.

$$\frac{d}{dt} e_\Phi(u|u_\infty) = -I_\Phi(u|u_\infty) \quad \text{and} \quad e_\Phi(u|u_\infty) \leq \frac{1}{2\omega} I_\Phi(u|u_\infty)$$

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Csiszar-Kullback inequality: $\|u - v\|^2_{L^1(\mathbb{R}^d)} \le C e_\Phi(u|v)$ if $u \ge 0$, $v \ge 0$ and $\int u = \int v$.

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**Theorem**

*$\Phi$ admissible entropy generator, $A$ $\omega$-convex, $u \ge 0$, $\int u_I \, dx = \int e^{-A} \, dx$, $e_\Phi(u_I|u_\infty) < \infty$. Then*

$$e_\Phi(u(t)|u_\infty) \le \exp(-2\omega t) e_\Phi(u_I|u_\infty)$$
$$\|u(t) - u_\infty\|_{L^1(\mathbb{R}^d)} \le C \exp(-\omega t) \ .$$

*References: D. Bakry + M. Emery 1984-1991, A.Arnold+P.Markowich+G.Toscani+A.Unterreiter, 2001.*

The entropy decay estimate is sharp.

# important examples of entropies:

- Boltzmann entropy: $\Phi(s) = s \ln s - s + 1$

decay estimate: $$\int_{\mathbb{R}^d} u(t) \ln\left(\frac{u(t)}{u_\infty}\right) dx \le e^{-2\omega t} \int_{\mathbb{R}^d} u_I \ln\left(\frac{u_I}{u_\infty}\right) \, dx$$

special case: $A(x) = \frac{\omega}{2}|x|^2 + c \Rightarrow$
$u_\infty(x) = e^{-A(x)} = \left(\frac{\omega}{2\pi}\right)^{d/2} \exp\left(-\frac{\omega}{2}|x|^2\right)$

$$\int_{\mathbb{R}^d} f^2 \, \ln f^2 \, du_\infty \le \frac{2}{\omega} \int_{\mathbb{R}^d} |\nabla f|^2 \, du_\infty + \|f\|^2_{L^2(du_\infty)} \ln \|f\|^2_{L^2(du_\infty)}$$

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- quadratic entropy generator $\Phi(s) = \frac{1}{2}(s-1)^2 \Rightarrow$ Poincaré inequality.

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- "intermediate" entropies: $\Phi(s) \sim s^p$, $1 < p < 2$!

# Extensions of the Theorem

- linear scalar Fokker-Planck equations:

$$u_t = \mathrm{div}\Big( \underbrace{D(x)}_{\text{unif. pos. def.}} \big(\nabla u + u \nabla (A(x) + \underbrace{B(x)}_{\in L^\infty(\mathbb{R}^d)} )\big)\Big)$$

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- nonlinear diffusion

$$u_t = \mathrm{div}(\nabla f(u) + u\nabla A(x))\ , \quad \text{e.g.} \quad f(u) = u^m$$

fast diffusion, porous media flows, ...
F.Otto 1999: gradient flow w.r.t. Wasserstein metric
J.Carillo+A.Jüngel+P.Markowich+G.Toscani+A.Unterreiter 2001

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$$u_t = \mathrm{div}(\nabla u + u \nabla A(x;\xi;u)) \text{ on } \mathbb{R}^d\,,\ t > 0\,; \quad u(t=0) = u_I(x,\xi)$$

$u = u(x;\xi;t)$...oscillator density, $\xi \in \mathbb{R}^M$ ...parameter representing interaction noise.

$$A(x;\xi;u) := \omega\frac{|x|^2}{2} + \frac{\Theta}{2}|z_u - x|^2 - x \cdot \sum_{l,m=1}^{M} s_{u,m} E_{l,m} \xi_l + \frac{1}{2}\sum_{l,m=1}^{M} E_{l,m} s_{u,l} \cdot s_{u,m}$$

$\omega\frac{|x|^2}{2}$ ...single oscillator potential
$\Theta$ ... interaction strength $> 0$
$E = (E_{l,m})$...positive definite symmetric matrix

$dP(\xi)$: probability distribution of the noise vector $\xi \in \mathbb{R}^M$

$$z_u := \int_{\mathbb{R}^M_\xi}\int_{\mathbb{R}^d_x} x u(x,\xi)\, dx\, dP(\xi)$$

$$s_{u,l} := \int_{\mathbb{R}^M_\xi}\int_{\mathbb{R}^d_x} x \xi_l u(x,\xi)\, dx\, dP(\xi)$$

averages, source of the nonlinear convection

$$u_0(x;\xi;u(t)) := c(\xi)\ \exp(-A(x;\xi;u(t)) \ldots$$

...intermediate asymptotic state (candidate)

$$u_t = \operatorname{div}\left(u_0 \nabla\left(\frac{u}{u_0}\right)\right) \Big| \quad \cdot \ln\left(\frac{u}{u_0}\right) \ , \quad \iint \cdot \, dx\, dP(\xi)$$

attention: $u_0$ depends on $t$!!

$$\frac{d}{dt}\underbrace{\int_{\mathbb{R}^M_\xi}\int_{\mathbb{R}^d_x} u \ln\left(\frac{u}{u_0}\right) dx\, dP(\xi)}_{e(u|u_0)} = -\underbrace{\int_{\mathbb{R}^M_\xi}\int_{\mathbb{R}^d_x} u \left|\nabla\left(\frac{u}{u_0}\right)\right|^2 dx\, dP(\xi)}_{I(u|u_0)}$$

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## Theorem

*(Arnold+Markowich+Toscani+Unterreiter, 2001): Let* $E \leq e_0 I$, $\gamma := \int_{\mathbb{R}^M} |\xi|^2\, dP(\xi)$ *and assume that* $\lambda := \omega - e_0\gamma > 0$. *Define* $u_\infty(x,\xi) := N \exp(-(\frac{\omega}{2} + \frac{\Theta}{2})|x|^2) \int_{\mathbb{R}^m} u_I(x,\xi)\, dx$. *Then*

$$\|u(t) - u_\infty\|_{L^1(dx\, dP(\xi))} = O(e^{-\lambda t})\ .$$

# Degenerate Quasilinear Diffusive Systems

A. Jüngel+P. Markowich+G. Toscani, 2001

$u = u(x,t) : \mathbb{R}_x^d \times \mathbb{R}_t^+ \mapsto \mathbb{R}^N$...vector of unknowns

$$\begin{cases} \dfrac{\partial}{\partial t} b(u) - \operatorname{div} a(u, \nabla u) = f(u) & \text{in} \quad \mathbb{R}_x^d \times \mathbb{R}_t^+ \\ b(u(x, t=0)) = b(u_I(x)) & \text{in} \quad \mathbb{R}_x^d \end{cases}$$

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- $b : \mathbb{R}^N \to \mathbb{R}^N$, $b = \nabla \chi$ with $\chi(0) = 0$ and $\beta$ is strictly monotone: $\exists \beta, B, m > 0$: $\beta |u - v|^{1+\frac{1}{m}} \leq (b(u) - b(v)) \cdot (u - v) \leq B |u - v|^{1+\frac{1}{m}}$ $\forall u, v \in \mathbb{R}^N$.

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- $b : \mathbb{R}^N \to \mathbb{R}^N$, $b = \nabla \chi$ with $\chi(0) = 0$ and $\beta$ is strictly monotone: $\exists \beta, B, m > 0$: $\beta |u - v|^{1+\frac{1}{m}} \leq (b(u) - b(v)) \cdot (u - v) \leq B|u - v|^{1+\frac{1}{m}}$ $\forall u, v \in \mathbb{R}^N$.
- $a : \mathbb{R}^N \times \mathbb{R}^{N \times d} \mapsto \mathbb{R}^{N \times d}$, $a(u, 0) = 0 \ \forall u \in \mathbb{R}^N$ and $a$ is elliptic: $\exists \alpha > 0, p \geq 2$: $(a(u, z_1) - a(u, z_2)) : (z_1 - z_2) \geq \alpha |z_1 - z_2|^p$ $\forall u \in \mathbb{R}^N$; $z_1, z_2 \in \mathbb{R}^{N \times d}$.

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A. Jüngel+P. Markowich+G. Toscani, 2001
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$$\begin{cases} \frac{\partial}{\partial t} b(u) - \operatorname{div} a(u, \nabla u) = f(u) & \text{in} \quad \mathbb{R}^d_x \times \mathbb{R}^+_t \\ b(u(x, t=0)) = b(u_I(x)) & \text{in} \quad \mathbb{R}^d_x \end{cases}$$

- $b : \mathbb{R}^N \to \mathbb{R}^N$, $b = \nabla \chi$ with $\chi(0) = 0$ and $\beta$ is strictly monotone: $\exists \beta, B, m > 0$: $\beta |u - v|^{1+\frac{1}{m}} \leq (b(u) - b(v)) \cdot (u - v) \leq B|u - v|^{1+\frac{1}{m}}$ $\forall u, v \in \mathbb{R}^N$.
- $a : \mathbb{R}^N \times \mathbb{R}^{N \times d} \mapsto \mathbb{R}^{N \times d}$, $a(u, 0) = 0 \; \forall u \in \mathbb{R}^N$ and $a$ is elliptic: $\exists \alpha > 0, p \geq 2$: $(a(u, z_1) - a(u, z_2)) : (z_1 - z_2) \geq \alpha |z_1 - z_2|^p$ $\forall u \in \mathbb{R}^N$; $z_1, z_2 \in \mathbb{R}^{N \times d}$.
- $f : \mathbb{R}^N \mapsto \mathbb{R}^N$, $f(u) \cdot u \leq 0$, $\forall u \in \mathbb{R}^N$.

$$0 \leq e(u) := b(u) \cdot u - \chi(u) \quad \text{...Legendre transform of } \chi$$

$$E(u) := \int_{\mathbb{R}^d} e(u)\, dx \quad \text{...entropy functional, H. Alt+S.Luckhaus, 1989}$$

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$$\leq -\alpha \int_{\mathbb{R}^d} |\nabla u|^p\, dx \leq -c \|u\|^{p(1+\sigma)}_{L^{1+\frac{1}{m}}} \quad \text{if } b(u) \in L^\infty_t(L^1_x)$$

generalized Nash inequality: $\|w\|^{1+\sigma}_{L^{1+\frac{1}{m}}} \leq \Gamma \| |w|^{1/m} \|^{\sigma m}_{L^1} \|\nabla w\|_{L^p}$ for $m > \frac{1}{2}$, $p \geq 1,\ p > \frac{d(m+1)}{dn+m+1}$, $\sigma = \sigma(d, m, p) > 0$.

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generalized Nash inequality: $\|w\|_{L^{1+\frac{1}{m}}}^{1+\sigma} \leq \Gamma \||w|^{1/m}\|_{L^1}^{\sigma m} \|\nabla w\|_{L^p}$ for $m > \frac{1}{2}$, $p \geq 1,\ p > \frac{d(m+1)}{dn+m+1}$, $\sigma = \sigma(d, m, p) > 0$.

also: $E(u) \leq c_1 \|u\|_{L^{1+\frac{1}{m}}}^{1+\frac{1}{m}} \Rightarrow \underline{\frac{d}{dt}E \leq -c_2 E^{1+\delta}}$, $c_2 > 0,\ d > 0$.

## Theorem

*(Jüngel+Markowich+Toscani, 2001): Let* $b(u) \in L^\infty_t(L^1_x)$, $m > \frac{1}{2}$ *and* $p > \frac{d(m+1)}{dm+1}$. *Then*

$$\exists \delta > 0, C > 0 : \begin{array}{l} E(u(t)) \leq (E(u_I)^{-\delta} + \delta C t)^{-\frac{1}{\delta}} \\ \|u(t)\|_{L^{1+\frac{1}{m}}} \leq C(E(u_I)^{-\delta} + \delta C t)^{-\frac{m}{\delta(m+1)}} \end{array}$$

$$\text{and, if} \quad m > 1 \ : \quad \|u(t)\|_{L^1} \leq C(E(u_I)^{-\delta} + \delta C t)^{-\frac{m-1}{\delta m}} \ ,$$

$$\text{where} \quad \delta = \frac{dm(p-1) + p - d}{dm} > 0 \ .$$

Note: There is -so far- no general existence-uniqueness result.

Examples: $N = 1$ (scalar case), $b(u) = |u|^{\frac{1}{m}-1}u$, $a(u,z) = |z|^{p-2}z$

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# Confined vs. unconfined Diffusion

$$u_t = \mathrm{div}(\nabla(u^m) + xu) \quad \text{in} \quad \mathbb{R}^d_x \times \mathbb{R}^+_t \quad \text{confinement potential: } V(x) = \frac{1}{2}|x|^2$$

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spatio-temporal rescaling: $(x, t) \leftrightarrow (y, \tau)$

$$\left\| \begin{array}{l} \tau = \dfrac{1}{2-d+dm}(\exp((2-d+dm)t) - 1) \\ y = R(\tau)x \ , \quad R(\tau) := ((2-d+dm)\tau + 1)^{\frac{1}{2-d+dm}} \end{array} \right\| \quad m > \frac{d-2}{d}!!!$$

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$$\left.\begin{array}{l} \text{exponential convergence as } t \to \infty \\ \text{to } u = 0 \text{ for confined solutions} \end{array}\right\} \Leftrightarrow \left\{\begin{array}{l} \text{algebraic convergence as } t \to \infty \\ \text{to } v = 0 \text{ for unconfined solutions} \end{array}\right.$$

# Reaction-Diffusion Systems: Turing Instability

Scalar case:

$$u_t = \Delta u + f(u) \quad \text{subject to hom. Neumann b.cs.}$$

.

Assume: $f(0) = 0$, $f'(0) < 0 \Rightarrow \frac{d}{dt}u = f(u)$ is linearly stable at $u = 0$.

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"morally": in the scalar case diffusion does not change (linearized) stability!

and - at least locally close to the steady state $u_\infty \equiv 0$ - linearized stability implies nonlinear stability.

# Systems of 2 Reaction-Diffusion Equations

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}_t = \begin{pmatrix} \Delta u_1 \\ D\Delta u_2 \end{pmatrix} + \begin{pmatrix} f(u_1, u_2) \\ g(u_1, u_2) \end{pmatrix}$$ subject to hom. Neumann b.cs.

assume: $f(0,0) = g(0,0) = 0$ and the homogeneous system

$$\frac{d}{dt}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} f(u_1, u_2) \\ g(u_1, u_2) \end{pmatrix}$$

is linearly stable, i.e. $B = \begin{pmatrix} f_{u_1}(0,0) & f_{u_2}(0,0) \\ g_{u_1}(0,0) & g_{u_2}(0,0) \end{pmatrix}$ is negativ definit, but not symmetric.

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A. Turing 1952: There are systems with the properties stated above such that if $D$ is sufficiently different from 1, the linearized problem $\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_t = \begin{pmatrix} \Delta v_1 \\ D\Delta v_2 \end{pmatrix} + B\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ is unstable!!

"morally": large differences in the diffusivities may lead to departure from the equilibrium state

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$\Rightarrow$ pattern formation for activator-inhibitor reaction-diffusion systems.

# Stable Linear Diffusion-Reaction Systems: Entropy

$$\begin{cases} U_t = \mathrm{div}(D(x)\nabla U(x)) + R(x)U(x)\,, \quad x \in G \text{ bdd. in } \mathbb{R}^d\,, \quad t > 0 \\ D(x)\nabla U(x) n(x) = 0 \quad \text{on} \quad \partial G\,, \quad t > 0 \\ U(x, t = 0) = U_I(x) \end{cases}$$

$U_I, U \in \mathbb{R}^N$; $D, R$...real $N \times N$-matrices.

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structure assumptions

1. $\exists\ S \in \mathbb{R}^{N\times N}$ constant, symmetric, pos. definite s.t.:

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2. $\exists E \in \mathbb{R}^{N \times N}$ constant, orthogonal, $E^j$: j-th row-vector of $E$:

$$E\tilde{R}(x)E^T = \mathrm{diag}(\underbrace{0, ..., 0}_{n}, \lambda_{n+1}(x), ..., \lambda_N(x))\,, \quad \lambda_i(x) \leq -\underline{\lambda} < 0$$

The zero eigenvalues of $R$ correspond to conservation laws:

### Lemma

*For $j = 1, .., n$ the quantitiy $I_j := \int_G E^j SU(x,t)\, dx$ is time-conserved.*

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**Lemma**

*For given $(I_1, ..., I_n) \in \mathbb{R}^n$ $\exists!$ equilibrium state $U_\infty$ s.t. $U_\infty$ is a constant vector and $I_j = \mathrm{vol}(G) E^j SU^\infty$, $j = 1, ..., n$ (effect of diffusion) $(EU^\infty)_j = 0$, $j = n+1, ..., N$ (effect of reaction).*

"morally": both diffusion and reaction dissipate the energy $E[U]$.

BUT: diffusion drives $U$ towards its mean-value $\frac{1}{|G|}\int_G U\,dx$ as $t \to \infty$, while reaction drives $U$ towards the linear space $R(x)U = 0$ as $t \to \infty$.

Thus: there is no full 'cooperation' between diffusion and reaction in the long-time asymptotics.

### Theorem

*(Di Francesco+Fellner+Markowich 2007) Define:*

$$I_j := \int_G E^j S U_I(x)\,dx\ , \quad j = 1, \dots, n\ .$$

*Then* $\exists\ K > 0$*:*

$$E[U(t) - U_\infty] = O(e^{-Kt})\,.$$

*Remark: the rate $K$ is generally smaller than the sum of the individual diffusion and reaction dissipation rates!!*

# Stable Nonlinear Reaction-Diffusion Systems: Entropy

- A. Glitzky+K. Gröger+R.Hünlich 1995: semiconductor drift-diffusion model on bdd. domain, $t \to \infty$ asymptotics.
- A. Arnold+P.Markowich+G.Toscani, 2001: semiconductor drift diffusion model, log-Sobolev inequality.
- H.Wu+P.Markowich+S.Zeng 2007: semiconductor drift-diffusion model: existence, $t \to \infty$ asymptotics
- M. Di Francesco+K.Fellner+P.Markowich: semiconductor drift diffusion model: exponential convergence as $t \to \infty$ (work in progress!)
- B. Perthame, J. Dolbeault 2005: entropy techniques for various PDEs in cell and population biology.
- L. Desvillettes + K.Fellner 2006, L.Desvillettes + K.Fellner + M.Pierre + J.Vovelle 2006: chemical kinetics RD-systems, bounded domain: logarithmic Boltzmann entropy, existence+exponential convergence

# The Drift-Diffusion Semiconductor Model

$$\left.\begin{aligned} n_t &= \operatorname{div}(\nabla n + n\nabla(\psi + A(x))) - R(n,p,x) \\ p_t &= \operatorname{div}(\nabla p + p\nabla(-\psi + A(x))) - R(n,p,x) \\ -\Delta\psi &= n - p - D(x) \end{aligned}\right\} x \in G\ , \quad t > 0$$

$$\left.\begin{aligned} &n\text{...electron position density}, \geq 0 \\ &p\text{...hole position density}, \geq 0 \\ &\psi\text{...electric potential} \end{aligned}\right\} \text{unknowns}$$

$D(x)$... doping profile (determining the device)
for simplicity: $G = \mathbb{R}^3$, $A = A(x)$...confining potential
$R(n,p,x) = \underbrace{F(n,p,x)}_{>0}(np - e^{-2A(x)})$...recombination-generation rate.

- van Roosbrook ∼50: derivation of the PDE system
- M. Sever ∼70-80: existence, uniqueness issues
- P.Markowich ∼80: qualitative +quantitative analysis, Springer book, 1986
- P.Markowich+C.Ringhofer+C.Schmeiser: Springer book, 1993
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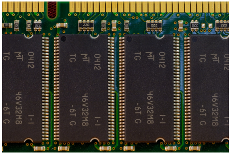

Remarks

- the DD semiconductor model has been the basis for industrial semiconductor design since 1970 ...and it still is...
- system of two diffusion-convection-reaction equations, nonlinearly coupled by the reaction term and by the nonlocally defined Coulomb potential
- set $p \equiv 0$, $R \equiv 0$, $D \equiv 0$, replace $\Delta\psi$ by $-\Delta\psi \Rightarrow$ Keller-Segel system for chemotaxis!!!

Assumptions:

1. $A(x)$ is $\sigma-$convex, i.e. $D^2A(x) \geq \sigma I \ \forall \ x \in \mathbb{R}^3$, $\Delta A \in L^\infty(\mathbb{R}^3)$, $\mu := e^{-A}$, $\int_{\mathbb{R}^3} \mu \, dx = 1$

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3. $R$ is smooth, $|R(n,p,x)| \leq C(a(x) + |n| + |p|)$, $a \in L^1_+ \cap L^\infty(\mathbb{R}^3)$, $a\sqrt{\mu} \in L^2(\mathbb{R}^3)$
   typical form: $R = (np - \mu^2)/(r_1(x) + r_2(x)n + r_3(x)p)$ with $r_i > 0$.
   Shockley-Read-Hall recombination-generation rate

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4. $n(t=0) = n_I$, $p(t=0) = p_I$; $n_I, p_I \in L^4_+(\mathbb{R}^3) \cap L^2(e^A dx)$

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   Shockley-Read-Hall recombination-generation rate
4. $n(t=0) = n_I$, $p(t=0) = p_I$; $n_I, p_I \in L^4_+(\mathbb{R}^3) \cap L^2(e^A dx)$

charge conservation:

$$\int_{\mathbb{R}^3} (n(x,t) - p(x,t) - D(x)) \, dx \equiv \int_{\mathbb{R}^3} (n_I - p_I - D) \, dx =: \alpha \ \forall t > 0$$

Assumptions:

1. $A(x)$ is $\sigma-$convex, i.e. $D^2A(x) \geq \sigma I \ \forall \ x \in \mathbb{R}^3$, $\Delta A \in L^\infty(\mathbb{R}^3)$, $\mu := e^{-A}$, $\int_{\mathbb{R}^3} \mu \, dx = 1$
2. $D \in L^1 \cap L^\infty(\mathbb{R}^3)$
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**Theorem**

*(H.Wu, P.Markowich, S.Zheng 2007): the DD system admits a unique global smooth solution* $(n,p) \in \mathcal{C}([0,\infty); L^2(e^A dx))^2$ *if (1)-(4) hold.*

# Equilibrium States

$$\left.\begin{aligned} 0 &= \mathrm{div}(\nabla n + n\nabla(\psi + A(x))) - F(n,p,x)(np - \mu^2) \\ 0 &= \mathrm{div}(\nabla p + p\nabla(-\psi + A(x))) - F(n,p,x)(np - \mu^2) \\ -\Delta\psi &= n - p - D(x) \end{aligned}\right\}$$

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Poisson equation: $-\Delta\psi_\infty = C_n[\psi_\infty] e^{-\psi_\infty}\mu - C_p[\psi_\infty] e^{\psi_\infty}\mu - D(x)$
...mean field equation

## Theorem

*(Wu+Markowich+Zheng 2007): There is a unique solution* $\psi_\infty \in L^6(\mathbb{R}^3)$, $\nabla\psi_\infty \in L^2(\mathbb{R}^3)$ *of the mean-field equation.*

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<u>Definition of the relative entropy</u>:

$$0 \le e(t) := \int_{\mathbb{R}^3} \left( n \left( \ln \frac{n}{n_\infty} - 1 \right) + n_\infty \right) dx \quad + \quad \int_{\mathbb{R}^3} \left( p \left( \ln \frac{p}{p_\infty} - 1 \right) + p_\infty \right) dx \, + \\ + \quad \frac{1}{2} \int_{\mathbb{R}^3} |\nabla\psi - \nabla\psi_\infty|^2 dx$$

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$$\frac{d}{dt} e(t) = \underbrace{- \int_{\mathbb{R}^3} n \left| \nabla \left( \frac{n}{N} \right) \right|^2 dx - \int_{\mathbb{R}^3} p \left| \nabla \left( \frac{p}{P} \right) \right|^2 dx - \overbrace{\int_{\mathbb{R}^3} F(n,p,x)(np - \mu^2) \ln \frac{np}{\mu^2} dx}^{\ge 0}}_{I} \le 0$$

$$N = C_n[\psi_\infty] e^{-\psi(t)} \mu \,, \quad P = C_p[\psi_\infty] e^{\psi(t)} \mu$$

# Convergence to Equilibrium

## Theorem

*(Wu+Markowich+Zheng) The global transient solution converges (in an appropriate sense) to the corresponding equilibrium.*

Proof: $e(t) \leq e(0) \Rightarrow n(t)|\ln n(t)| + n(t)(A(x)+1) \in L^1_x(\mathbb{R}^3)$ unif. in $t > 0 \Rightarrow$ (Dunford-Pettis) $n(., t_k + .)$ is weak-$L^1(\mathbb{R}^3 \times [0,S])$ compact for every sequence $t_k \to \infty$. Compactness for the identification of the weak limit of the time-shifted solutions is obtained from the bound of the entropy dissipation:

$$\int_0^\infty I(s)\,ds < \infty \Rightarrow \int_{t_k}^{t_k+S} I(s)\,ds = \int_0^S I(t_k+s)\,ds \stackrel{t_k\to\infty}{\longrightarrow} 0\,.$$

# Exponential Convergence

.... under construction .....

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.... under construction .....

Thank you for your attention!