On a problem of singular limits

Jean DOLBEAULT

Ceremade, Université Paris IX-Dauphine,
Place de Lattre de Tassigny,
75775 Paris Cédex 16, France

E-mail: dolbeaul@ceremade.dauphine.fr

`http://www.ceremade.dauphine.fr/~dolbeaul/`

Results obtained in collaboration with:
Caffarelli, Markowich & Schmeiser / Markowich & Unterreiter

$\Omega \in \mathbb{R}^d$, $C(x) \in L^\infty(\Omega)$
A model arising in semiconductor theory

Global electroneutrality

$$N - P - \int_\Omega C(x)\,dx = 0$$

Distribution of negatively / positively charged particles
$n(x) = N \frac{e^\phi}{\int_\Omega e^\phi\,dx}$, $p(x) = P \frac{e^{-\phi}}{\int_\Omega e^{-\phi}\,dx}$
Poisson equation

$$\boxed{\varepsilon \Delta \phi = n - p - C \quad \text{in } \Omega}$$

with Neumann boundary conditions ($\Leftrightarrow$ global electroneutrality)

$$\partial_\nu \phi = 0 \quad \text{on } \partial\Omega$$

Local electroneutrality

$$n - p - C = 0 \Rightarrow N - \int_\Omega C^+\,dx \geq 0 \Leftrightarrow P - \int_\Omega C^-\,dx \geq 0$$

A. Existence, uniqueness, uniform estimates ($\varepsilon > 0$)

Space: $\{\psi \in H^1(\Omega) \ : \ \int_\Omega \psi \, dx = 0\}$
Functional

$$J[\psi] = \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\psi|^2 - C\psi\right) dx + N \ln\left(\int_\Omega e^{\psi} dx\right) + P \ln\left(\int_\Omega e^{-\psi} dx\right)$$

J convex, coercive, $\log \int_\Omega e^{\psi} dx \geq C\|\nabla\psi\|_{L^2}$

Theorem 1 $C \in L^\infty(\Omega)$, $|\Omega| < +\infty$, $\partial\Omega \in C^1$
$\exists! \psi \in W^{2,p}(\Omega)$ *solution of the Poisson equation (unique: up to an additive constant)*

Intrinsic density: choose the constant such that

$$n_i = \frac{N}{\int_\Omega e^{\phi} \, dx} = \frac{P}{\int_\Omega e^{-\phi} \, dx}$$

Proposition 2 *n and p are uniformly bounded in $L^\infty(\Omega)$*

Proof. maximum of ϕ: $t = e^{-\phi}$

$$0 \geq n_i(t - \frac{1}{t}) - \bar{C} \Rightarrow t \leq \frac{\bar{C} + \sqrt{\bar{C}^2 + 4\,n_i}}{2\,n_i}$$

Let $\Omega_1 = \{x \in \Omega \ : \ \phi(x) \geq 0\}$, $\Omega_2 = \{x \in \Omega \ : \ \phi(x) \leq 0\}$. Then

$$n_i \leq \min\left(\frac{N}{\int_{\Omega_2} e^{\phi}\,dx}, \frac{P}{\int_{\Omega_1} e^{-\phi}\,dx}\right) \leq \frac{2}{|\Omega|} \max(N, P)$$

□

Lemma 3 *Local electroneutrality $\Rightarrow \phi$ is uniformly (with respect to ε) bounded in $L^\infty(\Omega)$*

Proof.
$N = \int_{\Omega_1} n\, dx + \int_{\Omega_2} n\, dx \le n_i\, |\Omega| + \int_{\Omega_1} n\, dx$
$\int_{\Omega_1} p\, dx \le n_i\, |\Omega|$
$\int_{\Omega_1} C\, dx \le \int_{\Omega} C^+\, dx$
$0 \ge \varepsilon \int_{\Omega_1} \Delta\phi\, dx$
$\quad = \int_{\Omega_1} (n-p-C)\, dx \ge N - \int_{\Omega} C^+\, dx - 2n_i\, |\Omega|$
gives a lower bound on n_i □

B. First case: Local neutrality

Theorem 4 *If* $N - \int_\Omega C^+ dx \ge 0 \Leftrightarrow P - \int_\Omega C^- dx \ge 0$ *and if* $C \in H^1(\Omega)$*, then* $(n_\varepsilon, p_\varepsilon) \to (n_0, p_0)$ **-weakly in* $L^\infty(\Omega)$ *where* (n_0, p_0) *is such that*

$$n_0 - p_0 - C = 0$$

Proof.

$$\begin{aligned} \int (n-p-C)\varepsilon\Delta\phi\, dx &= \varepsilon \int (n+p)|\nabla\phi|^2\, dx \\ &\quad -\varepsilon \int \nabla\phi\cdot\nabla C\, dx \\ &= -\int (n-p-C)^2\, dx \end{aligned}$$

$$\int (n-p-C)^2\, dx + Cst\varepsilon \int |\nabla\phi|^2\, dx \le \varepsilon \int \nabla\phi\cdot\nabla C\, dx$$

□

Remark 5 $n_0 - p_0 - C = 0$
$n_0 = N \frac{e^{\phi_0}}{\int_\Omega e^{\phi_0}\, dx}$, $p_0 = P \frac{e^{-\phi_0}}{\int_\Omega e^{-\phi_0}\, dx}$

$$\frac{N}{\int_\Omega e^{\phi_0}\, dx} = \frac{P}{\int_\Omega e^{-\phi_0}\, dx}$$

Therefore

$$e^{\phi_0} = \frac{C + \sqrt{C^2 + 4\, n_i}}{2\, n_i}$$

Since

$$2N = \int_\Omega n_i e^{\phi_0}\, dx = \int_\Omega (C + \sqrt{C^2 + 4\, n_i})\, dx\ ,$$

n_i *is uniquely determined*

C. 2nd case: A double obstacle problem

Rescale the potential

$$\Delta\Phi = n - p - C\,, \quad \min\Phi = 0$$

$n(x) = N\,\frac{e^{\Phi/\varepsilon}}{\int_\Omega e^{\Phi/\varepsilon}\,dx}$, $p(x) = P\,\frac{e^{\Phi/\varepsilon}}{\int_\Omega e^{\Phi/\varepsilon}\,dx}$
Let $\bar\Phi = \max\Phi = \Phi(x_0)$. Using the uniform bound in $W^{1,\infty}$: $\bar\Phi - \Phi \leq L\,|x - x_0|$

$$\int_\Omega e^{(\bar\Phi-\Phi)/\varepsilon}\,dx \geq \int_\Omega e^{-L\,|x-x_0|/\varepsilon}\,dx \geq C\,\varepsilon^{2d}$$

$n \leq \frac{N}{C\,\varepsilon^{2d}}\,e^{(\bar\Phi-\Phi)/\varepsilon} \to 0$ if $\Phi < \bar\Phi$, thus leading to the double obstacle problem

$$\begin{array}{ll} n_0 = C\,, \quad p_0 = 0\,, \quad \Phi_0 = \bar\Phi\,, & \text{in } \Omega_+\,, \\ p_0 = -C\,, \quad n_0 = 0\,, \quad \Phi_0 = 0\,, & \text{in } \Omega_-\,, \\ n_0 = p_0 = 0\,, \quad \Delta\Phi_0 + C = 0\,, & \text{in } \mathcal{N}\,. \end{array}$$

with the additional condition

$$\int_{\Omega_+} C\,dx = N$$

Theorem 6 $\bar{\Phi} \mapsto \int_{\Omega_+} C\, dx$ *is monotone*

Corollary 7 *As* $\varepsilon \to 0$, $\Phi_\varepsilon \to \Phi_0$ *in* $C^1(\Omega)$, *where* Φ_0 *is the unique solution of the double obstacle problem*

D. Remarks

Remark 8 *Variational formulation*

$$J_\varepsilon(\Psi) = \varepsilon J\left(\frac{\Psi}{\varepsilon}\right) = \int_\Omega \left(\frac{1}{2}|\nabla\Psi|^2 - C\Psi\right) dx + \varepsilon N \log\left(\int_\Omega e^{\Psi/\varepsilon} dx\right) + \varepsilon P \log\left(\int_\Omega e^{-\Psi/\varepsilon} dx\right) .$$

Second term on the right hand side:

$$N \sup_\Omega \Psi + \varepsilon N \log\left(\int_\Omega \exp\left(\frac{\Psi - \sup_\Omega \Psi}{\varepsilon}\right) dx\right) ,$$

Formally passing to the limit in J_ε

$$J_0(\Psi) = \int_\Omega \left(\frac{1}{2}|\nabla\Psi|^2 - C\Psi\right) dx + N \sup_\Omega \Psi .$$

$0 = \frac{d}{d\mu} J_0(\mu\Psi_0)|_{\mu=1} = \int_\Omega \left(|\nabla\Psi_0|^2 - C\Psi_0\right) dx + N \sup_\Omega \Psi_0 = \sup_\Omega \Psi_0 \cdot (\int_{\Omega_+} C\, dx - N)$.

Remark 9 *Dual formulation*

$$J[\psi] = \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\psi|^2 - C\psi\right) dx$$
$$+N \ln\left(\int_\Omega e^{\psi} dx\right) + P \ln\left(\int_\Omega e^{-\psi} dx\right)$$

Since

$$\frac{\varepsilon}{2}\int_\Omega |\nabla\psi|^2\,dx$$
$$= -\varepsilon\int_\Omega \psi\Delta\psi\,dx - \frac{\varepsilon}{2}\int_\Omega |\nabla\psi|^2\,dx$$
$$= -\int_\Omega (n-p-C)\,\psi\,dx - \frac{\varepsilon}{2}\int_\Omega |\nabla\psi|^2\,dx\ ,$$

and since for a solution

$n = N\,\frac{e^\psi}{\int_\Omega e^\psi\,dx} \Rightarrow \psi = \log n - \log N - \log \int_\Omega e^\psi\,dx$,

$J[\psi] = -E[n,p]$ *with*

$$E[n,p] = \int_\Omega \left(n\,\log(\frac{n}{N}) + p\,\log(\frac{p}{P}) + \frac{\varepsilon}{2}|\nabla\psi|^2\right)\,dx$$

E. Nonlinear diffusions

$$\begin{array}{l} n_t = \nabla \cdot (\nabla f(n) - n \nabla \phi) \\ p_t = \nabla \cdot (\nabla f(p) + p \nabla \phi) \\ \varepsilon \Delta \phi = n - p - C \end{array}$$

No flux + Neumann boundary conditions

$(\nabla f(n) - n \nabla \phi) \cdot \nu = (\nabla f(p) + p \nabla \phi) \cdot \nu = \nabla \phi \cdot \nu = 0$

Global electroneutrality

$$N - P - \int_\Omega C(x)\, dx = 0$$

[Gajewski], [Arnold, Markowich, Toscani], [Arnold, Markowich, Toscani, Unterreiter], [Biler, J.D.], [Biler, J.D., Markowich]

[Del Pino, J.D.], [Carrillo, Toscani], [Otto], [Carrillo, Juengel, Markowich, Toscani, Unterreiter]

$h(u) = \frac{f'(u)}{u}$, $g = h^{-1}$, h is the enthalpy
Stationary solution

$$n = g(\alpha[\phi] + \phi)\ , \quad p = g(\beta[\phi] - \phi)$$

$\alpha[\phi]$ and $\beta[\phi]$ are the Fermi levels given by the conditions

$$N = \int_\Omega g(\alpha[\phi] + \phi)\, dx\ , \quad P = \int_\Omega g(\beta[\phi] - \phi)\, dx$$

nonlinear Poisson equation

$$\boxed{\varepsilon \Delta \phi = g(\alpha[\phi] + \phi) - g(\beta[\phi] - \phi) - C(x)}$$

A convex functional

$$\begin{aligned} J[\phi] = \ & \tfrac{\varepsilon}{2} \textstyle\int_\Omega |\nabla \phi|^2\, dx + \int_\Omega G(\alpha[\phi] + \phi)\, dx \\ & + \textstyle\int_\Omega G(\beta[\phi] - \phi)\, dx - N\beta[\phi] - P\alpha[\phi] \end{aligned}$$

Better: let $H(u) = u\, h(u) - f(u)$ be a primitive of h and consider the convex functional

$$E[n,p] = \int_\Omega H[n]\, dx + \int_\Omega H[p]\, dx + \frac{\varepsilon}{2} \int_\Omega |\nabla \phi|^2\, dx$$

with the constraints

$$\int_\Omega n\, dx = N \quad \text{and} \quad \int_\Omega p\, dx = P$$

General case can essentially be reduced to the following abstract result

Theorem 10 $(\mathcal{B}, \|\cdot\|)$ *Banach space,* $\mathcal{C} \subset \mathcal{B}$*,* $\mathcal{C} \neq \emptyset$*, convex, closed set,* $E, F : \mathcal{C} \to \mathbb{R} \cup \{\infty\}$ *with* $\inf_{\mathcal{C}} E < \infty, \inf_{\mathcal{C}} F < \infty$*. Let*

$$\mathcal{C}^* := \{x \in \mathcal{C} : E(x) < \infty\} .$$

For $\lambda \in \mathbb{R}^+$ *let* $x_\lambda \in \mathcal{C}$*. If*
1) x_λ *is a minimizer of* $E_\lambda := E + \lambda^{-1} F$ *in* $\mathcal{C}$*.*
2) $x_\lambda \rightharpoonup x_0$ *weakly in* $\mathcal{B}$ *as* $\lambda \to 0$*.*

Then
a) $\limsup_{\lambda \to 0} F(x_\lambda) \leq \inf_{\mathcal{C}^*} F$*.*
b) If F *is weakly lower sequentially continuous at* x_0*, then* $F(x_0) \leq \inf_{\mathcal{C}^*} F$*.*
c) If F *is weakly lower sequentially continuous at* x_0 *and if* $E(x_0) < \infty$*, then* x_0 *is a minimizer of* F *in* $\mathcal{C}^*$*, i.e.* $F(x_0) = \inf_{\mathcal{C}^*} F$*.*
d) If x^* *is a minimizer of* F *in* $\mathcal{C}^*$*, then*

$$\limsup_{\lambda \to 0} E(x_\lambda) \leq E(x^*).$$

e) If x^* *is a minimizer of* F *in* $\mathcal{C}^*$ *and if* E *is weakly lower sequentially continuous at* x_0*, then* $E(x_0) \leq E(x^*)$*.*

f) If E *and* F *are weakly lower sequentially continuous at* x_0 *and if* $E(x_0) < \infty$*, then* x_0 *is a minimizer of* F *in* $\mathcal{C}^*$ *whose "energy"* $E(x_0)$ *is less or equal the energy* $E(x^*)$ *of any minimizer* x^* *of* F *in* $\mathcal{C}^*$*.*