REDUCTION OF DIMENSION FOR THE SCHRÖDINGER-POISSON SYSTEM

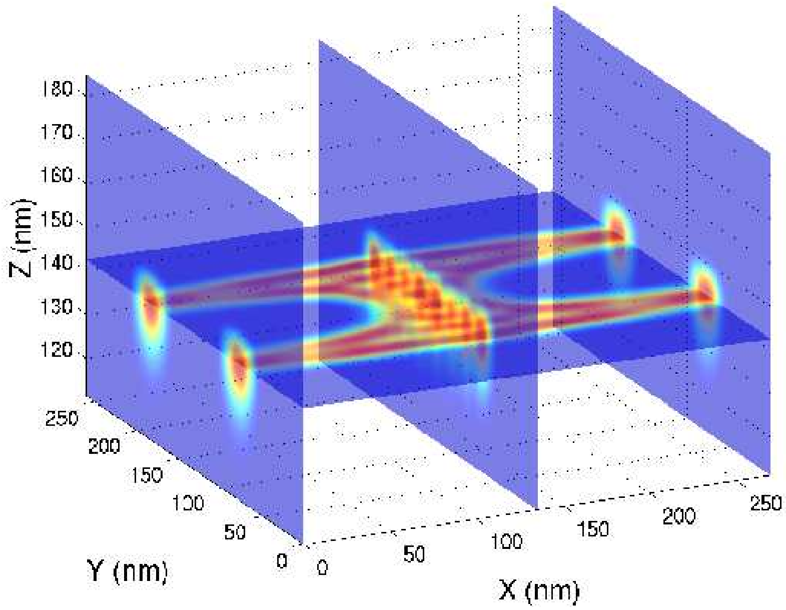
Florian Méhats

IRMAR, Univ. Rennes 1, France

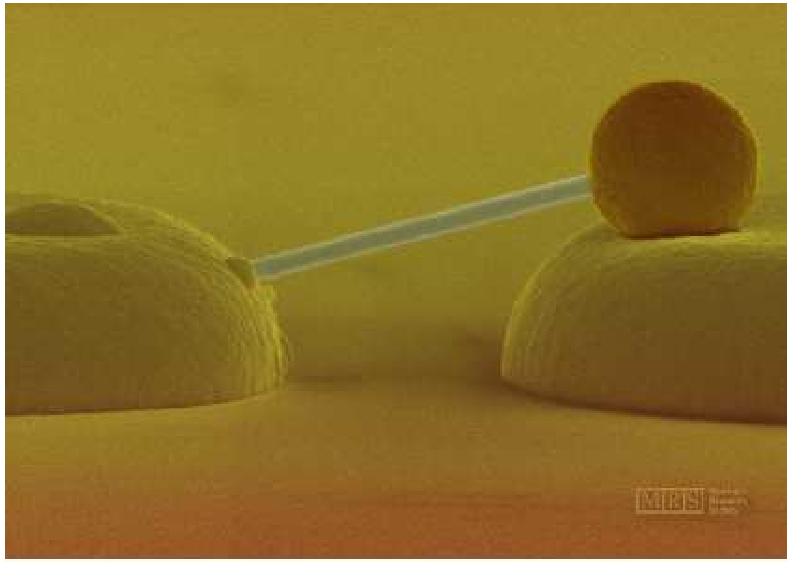
Collaborations with N. Ben Abdallah, F. Castella, F. Fendt, O. Pinaud

Workshop MESOTRANS 2008, Berlin

Derive models in reduced dimension for the transport of a quantum electron gas confined in a nanostructure.



Charge density in a quantum coupler



Silicom nanowire

1. Motivation

The gas is free to move in the transport directions $x \in \mathbb{R}^N$ but tightly confined in the transversal confinement directions $z \in \mathbb{R}^d$, $N + d = 3$.

Two situations :

- 2DEG = confinement on a plane, $N = 2,\ d = 1$, *e.g. layer on electrons in a MOSFET, on a graphene surface, in a quantum well,...*
- 1DEG = confinement on a line, $N = 1,\ d = 2$, *e.g. nanowire.*

Mathematical tool : asymptotic analysis for a singularly perturbed 3D Schrödinger-Poisson system.

Typical question : what is the form of the Poisson nonlinearity in the reduced model ?

Outline of the presentation

The singularly perturbed Schrödinger-Poisson system

$$i\partial_t \psi = -\Delta_x \psi - \Delta_z \psi + \frac{1}{\varepsilon^2} V_c\left(\frac{z}{\varepsilon}\right)\psi + V\psi$$

$$V = \frac{1}{4\pi\sqrt{|x|^2 + |z|^2}} * |\psi|^2$$

where V_c is a given smooth positive function and $V_c \to +\infty$ as $|z| \to +\infty$

The small parameter ε is the extension of the electron gas in the z direction.

The singularly perturbed Schrödinger-Poisson system

$$i\partial_t \psi = -\Delta_x \psi - \Delta_z \psi + \frac{1}{\varepsilon^2} V_c\left(\frac{z}{\varepsilon}\right)\psi + V\psi$$

$$V = \frac{1}{4\pi\sqrt{|x|^2 + |z|^2}} * |\psi|^2$$

where V_c is a given smooth positive function and $V_c \to +\infty$ as $|z| \to +\infty$

The small parameter ε is the extension of the electron gas in the z direction.

Rescaling (L^2 invariant) : $z' = \frac{z}{\varepsilon}\,, \qquad t' = t\,, \qquad x' = x$

$$\psi(t, x, z) = \frac{1}{\varepsilon^{d/2}}\,\psi'\left(t, x, \frac{z}{\varepsilon}\right)$$

THE RESCALED SYSTEM

$$i\partial_t \psi^\varepsilon = -\Delta_x \psi^\varepsilon + \frac{1}{\varepsilon^2}\mathcal{H}_z \psi^\varepsilon + V^\varepsilon \psi^\varepsilon \quad \text{with} \quad \mathcal{H}_z = -\Delta_z + V_c$$

$$V^\varepsilon = \frac{1}{4\pi\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |\psi^\varepsilon|^2$$

Initial data : $\psi(t=0) = \psi_0$ in the energy space

$$\mathbb{H} = \left\{ u \in H^1(\mathbb{R}^3) \text{ such that } \sqrt{V_c}\, u \in L^2(\mathbb{R}^3) \right\}$$

Qualitative behavior :

- oscillations in time coming from $i\partial_t = \frac{1}{\varepsilon^2}\mathcal{H}_z$
- the Poisson potential V^ε tends to be independent of z

The filtered system

It is convenient to filter out the oscillations in time and consider $\phi^\varepsilon = e^{it\mathcal{H}_z/\varepsilon^2}\psi^\varepsilon$

$$i\partial_t\phi^\varepsilon = -\Delta_x\phi^\varepsilon + e^{+it\mathcal{H}_z/\varepsilon^2}V^\varepsilon e^{-it\mathcal{H}_z/\varepsilon^2}\phi^\varepsilon$$

$$V^\varepsilon = \frac{1}{4\pi\sqrt{|x|^2+\varepsilon^2|z|^2}} * \left|e^{-it\mathcal{H}_z/\varepsilon^2}\phi^\varepsilon\right|^2$$

The filtered system

It is convenient to filter out the oscillations in time and consider $\phi^\varepsilon = e^{it\mathcal{H}_z/\varepsilon^2}\psi^\varepsilon$

$$i\partial_t\phi^\varepsilon = -\Delta_x\phi^\varepsilon + e^{+it\mathcal{H}_z/\varepsilon^2}V^\varepsilon e^{-it\mathcal{H}_z/\varepsilon^2}\phi^\varepsilon$$

$$V^\varepsilon = \frac{1}{4\pi\sqrt{|x|^2+\varepsilon^2|z|^2}} * \left|e^{-it\mathcal{H}_z/\varepsilon^2}\phi^\varepsilon\right|^2$$

$\varepsilon \longrightarrow 0$: one has to distinguish the 2DEG ($x \in \mathbb{R}^2$) and 1DEG ($x \in \mathbb{R}$) cases.

- 2DEG : $V^\varepsilon \sim \dfrac{1}{4\pi|x|} * \left|e^{it\mathcal{H}_z/\varepsilon^2}\phi^\varepsilon\right|^2$ which is well defined,
- 1DEG : problem since $\dfrac{1}{|x|}$ is not integrable !

Theorem. *Let* $\psi_0 \in \mathbb{H}$*. Then, as* $\varepsilon \to 0$*, the filtered function* ϕ^ε *converges locally uniformly in time in the* $\mathbb{H}$ *topology to the solution* ϕ *of the following system :*

$$i\partial_t \phi = -\Delta_x \phi + V\phi\,, \qquad \phi(t=0) = \psi_0\,,$$

$$V = \frac{1}{4\pi|x|} *_x \left\langle |\phi|^2 \right\rangle ,$$

where $\langle \cdot \rangle$ *denotes the integral over the transversal variable* $\int_{\mathbb{R}} \cdot dz$.

Theorem. *Let* $\psi_0 \in \mathbb{H}$*. Then, as* $\varepsilon \to 0$*, the filtered function* ϕ^ε *converges locally uniformly in time in the* $\mathbb{H}$ *topology to the solution* ϕ *of the following system :*

$$i\partial_t \phi = -\Delta_x \phi + V\phi\,, \qquad \phi(t=0) = \psi_0\,,$$

$$V = \frac{1}{4\pi|x|} *_x \left\langle |\phi|^2 \right\rangle,$$

where $\langle \cdot \rangle$ *denotes the integral over the transversal variable* $\int_{\mathbb{R}} \cdot dz$.

Remark. The dynamics is 2D, as expected, but the Poisson kernel is not the 2D Poisson kernel. It keeps track of the third dimension : if $u = u(x)$ then

$$\frac{1}{4\pi|x|} *_x u = \frac{1}{4\pi\sqrt{|x|^2 + |z|^2}} * \left(u(x)\delta_{z=0}\right)\Big|_{z=0}$$

Come-back to the initial function

The operator $\mathcal{H}_z$ has a discrete spectrum. Denote by $(E_p)_{p\in\mathbb{N}}$ its eigenvalues and by $(\chi_p)_{p\in\mathbb{N}}$ its eigenfunctions. The solution of the initial system (before rescaling and filtering) can be written asymptotically, as $\varepsilon \longrightarrow 0$,

$$\psi^\varepsilon(t,x,z) \sim \sum_{p=0}^{\infty} e^{-itE_p/\varepsilon^2}\,\phi_p(t,x)\,\frac{1}{\sqrt{\varepsilon}}\chi_p\left(\frac{z}{\varepsilon}\right),$$

where the ϕ_p's solve the following system :

$$i\partial_t\phi_p = -\Delta_x\phi_p + V\phi_p\,, \qquad \phi_p(t=0) = \int_{\mathbb{R}} \psi_0(x,z)\,\chi_p(z)\,dz\,,$$

$$V = \frac{1}{4\pi|x|} * \left(\sum_{p=0}^{\infty} |\phi_p|^2\right).$$

Write the system as a nonlinear Schrödinger equation

$$i\partial_t \phi^\varepsilon = -\Delta_x \phi^\varepsilon + G(\phi^\varepsilon), \qquad \phi^\varepsilon(t=0) = \psi_0\,,$$

where the nonlinearity is

$$G(u) = e^{+it\mathcal{H}_z/\varepsilon^2}\left(\left(\frac{1}{4\pi\sqrt{|x|^2+\varepsilon^2|z|^2}} * \left|e^{-it\mathcal{H}_z/\varepsilon^2}u\right|^2\right) e^{-it\mathcal{H}_z/\varepsilon^2}u\right).$$

Steps of the proof :

- an adapted functional framework based on $\mathcal{H}_z$,
- analysis of the nonlinearity and local in time estimates,
- energy estimate and global in time result.

Remark : no need to take time averages as in the talk of F. Castella (NLS).

STEP 1 : FUNCTIONAL FRAMEWORK ADAPTED TO THE HAMILTONIAN

Recall that $\mathcal{H}_z = -\partial_z^2 + V_c(z)$. We work in the scale of Sobolev spaces B^s, $s \in \mathbb{R}_+$ defined by the norm

$$\|u\|_{B^s} = \|u\|_{L^2} + \|(-\Delta_x)^{s/2} u\|_{L^2} + \|(-\mathcal{H}_z)^{s/2} u\|_{L^2}.$$

Practical use : $\mathcal{H}_z$ commutes with the rapidly oscillating operator $e^{+it\mathcal{H}_z/\varepsilon^2}$, which is unitary in any B^s (this “singular” operator become “transparent”).

Identification : (see talk of F. Castella) under some assumptions on V_c at the infinity –typically, symbol behavior– this norm is equivalent to

$$\|u\|_{H^s} + \|(V_c)^{s/2} u\|_{L^2}.$$

Case $B^1 = \mathbb{H}$ obvious. General case more difficult, requires Weyl-Hörmander pseudodifferential calculus (Helffer ’84, Bony-Chemin ’94, Helffer-Nier ’05).

STEP 2 : ANALYSIS OF THE STRENGTH OF THE NONLINEARITY IN B^s

Leading idea : the Poisson kernel behaves as the convolution with $\frac{1}{|x|}$, $x \in \mathbb{R}^2$.
Using Hardy-Littlewood-Sobolev estimates, we get

$$\|G(u)\|_{B^1} \leq C \, \|u\|_{B^1}^3 \, ,$$

and more generally the tame estimate, for any $s \geq 1$

$$\|G(u)\|_{B^s} \leq C \, \|u\|_{B^1}^2 \, \|u\|_{B^s} \, .$$

Consequences :

- estimate of ψ^ε in $\mathbb{H}$ independent of ε on a small time interval,
- if $\psi_0 \in B^s$, then estimate in B^s on the same time interval.

Step 3 : Asymptotic analysis of the Poisson kernel

$$\left\| \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |u|^2 \right) u - \left(\frac{1}{|x|} *_x \langle |u|^2 \rangle \right) u \right\|_{B^1} \leq C\, \varepsilon^{\alpha} \, \|u\|_{B^2}^3$$

with $0 < \alpha$ determined by the growth of V_c at the infinity.

Consequence :

$$G(u) = e^{+it\mathcal{H}_z/\varepsilon^2} \left(\left(\frac{1}{4\pi\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * \left| e^{-it\mathcal{H}_z/\varepsilon^2} u \right|^2 \right) e^{-it\mathcal{H}_z/\varepsilon^2} u \right).$$

Step 3 : Asymptotic analysis of the Poisson kernel

$$\left\| \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |u|^2 \right) u - \left(\frac{1}{|x|} *_x \langle |u|^2 \rangle \right) u \right\|_{B^1} \leq C\, \varepsilon^{\alpha} \, \|u\|_{B^2}^3$$

with $0 < \alpha$ determined by the growth of V_c at the infinity.

Consequence :

$$G(u) = e^{+it\mathcal{H}_z/\varepsilon^2} \left(\left(\frac{1}{4\pi |x|} *_x \left\langle \left| e^{-it\mathcal{H}_z/\varepsilon^2} u \right|^2 \right\rangle \right) e^{-it\mathcal{H}_z/\varepsilon^2} u \right) + \text{remainder}$$

Step 3 : Asymptotic analysis of the Poisson kernel

$$\left\| \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |u|^2 \right) u - \left(\frac{1}{|x|} *_x \langle |u|^2 \rangle \right) u \right\|_{B^1} \leq C\, \varepsilon^\alpha \, \|u\|_{B^2}^3$$

with $0 < \alpha$ determined by the growth of V_c at the infinity.

Consequence :

$$G(u) = \left(\left(\frac{1}{4\pi |x|} *_x \left\langle \left| e^{-it\mathcal{H}_z/\varepsilon^2} u \right|^2 \right\rangle \right) u \right) + \text{remainder}$$

Step 3 : Asymptotic analysis of the Poisson kernel

$$\left\| \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |u|^2 \right) u - \left(\frac{1}{|x|} *_x \langle |u|^2 \rangle \right) u \right\|_{B^1} \leq C\, \varepsilon^{\alpha}\, \|u\|_{B^2}^3$$

with $0 < \alpha$ determined by the growth of V_c at the infinity.

Consequence :

$$G(u) = \left(\left(\frac{1}{4\pi |x|} *_x \langle | \quad u|^2 \rangle \right) \quad u \right) + \text{remainder}$$

Then we obtain the convergence result by coupling these estimates and the nonlinear analysis for the Schrödinger-Poisson system (a regularization of the initial data is necessary in a step).

Step 4 : From local to global in time result

Notice that the energy conservation was useless to provide an estimate in $\mathbb{H}$.

The total energy is indeed the sum of the kinetic energy, the selfconsistent potential energy and the energy of the confinement, which is of order $1/\varepsilon^2$:

$$\|\nabla_x \psi^\varepsilon\|_{L^2}^2 + \|V^\varepsilon |\psi^\varepsilon|^2\|_{L^1} + \frac{1}{\varepsilon^2}\|\mathcal{H}_z^{1/2}\psi^\varepsilon\|^2 \text{ is conserved.}$$

STEP 4 : FROM LOCAL TO GLOBAL IN TIME RESULT

Notice that the energy conservation was useless to provide an estimate in $\mathbb{H}$.

The total energy is indeed the sum of the kinetic energy, the selfconsistent potential energy and the energy of the confinement, which is of order $1/\varepsilon^2$:

$$\|\nabla_x \psi^\varepsilon\|_{L^2}^2 + \|V^\varepsilon |\psi^\varepsilon|^2\|_{L^1} + \frac{1}{\varepsilon^2}\|\mathcal{H}_z^{1/2}\psi^\varepsilon\|^2 \text{ is conserved.}$$

However, the situation is different in the limit system, where a decoupling occurs :

$$\|\nabla_x \psi\|_{L^2}^2 + \|V|\psi|^2\|_{L^1} \text{ and } \frac{1}{\varepsilon^2}\|\mathcal{H}_z^{1/2}\psi\|^2 \text{ are \textbf{separately} conserved.}$$

Consequence : the limit system is globally well-posed and one can use the theorem of convergence in the energy space to prove that this convergence occurs on any arbitrary time interval.

Asymptotic result for the Poisson kernel if $x \in \mathbb{R},\ z \in \mathbb{R}^2$

For u in the energy space $\mathbb{H}$, one has

$$\left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |u|^2 \right) u = -2 \log \varepsilon \left\langle |u|^2 \right\rangle u + R^\varepsilon,$$

where $\|R^\varepsilon\|_{L^2} \leq C \|u\|_{\mathbb{H}}^3$.

Asymptotic result for the Poisson kernel if $x \in \mathbb{R},\ z \in \mathbb{R}^2$

For u in the energy space $\mathbb{H}$, one has

$$\left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |u|^2 \right) u = -2 \log \varepsilon \left\langle |u|^2 \right\rangle u + R^\varepsilon,$$

where $\|R^\varepsilon\|_{L^2} \leq C \|u\|_{\mathbb{H}}^3$.

Consequence 1 : in order to get a finite limit, one has to consider initial data of order $|\log \varepsilon|^{-1/2}$ or, equivalently, to work with the rescaled system

$$i\partial_t \psi^\varepsilon = -\Delta_x \psi^\varepsilon + \frac{1}{\varepsilon^2} \mathcal{H}_z \psi^\varepsilon + \frac{1}{|\log \varepsilon|} V^\varepsilon \psi^\varepsilon \qquad \psi^\varepsilon(t=0) = \psi_0$$

$$V^\varepsilon = \frac{1}{4\pi \sqrt{|x|^2 + \varepsilon^2 |z|^2}} * |\psi^\varepsilon|^2$$

Consequence 2 : the nonlinearity induces a "loss of derivative" :

instead of $\|G(u)\|_{B^1} \leq C\,\|u\|_{B^1}^3$, one has $\|G(u)\|_{B^1} \leq C\,\|u\|_{B^2}^3$.

$\Longrightarrow$ Lack of estimate.

Alternative proof : take advantage of the energy estimate for well-prepared initial data, polarized on the first eigenmode of $\mathcal{H}_z$.

By combining the equations of conservation of the charge and of conservation of the energy, one gets

$$\|\nabla_x\psi^\varepsilon(t)\|_{L^2}^2 + \frac{1}{|\log\varepsilon|}\left\|V^\varepsilon(t)|\psi^\varepsilon(t)|^2\right\|_{L^1} + \frac{1}{\varepsilon^2}\|(\mathcal{H}_z - E_0)^{1/2}\psi^\varepsilon(t)\|_{L^2}^2$$
$$= \|\partial_x\psi_0\|_{L^2}^2 + \frac{1}{|\log\varepsilon|}\left\|V^\varepsilon(0)|\psi_0|^2\right\|_{L^1} + \frac{1}{\varepsilon^2}\|(\mathcal{H}_z - E_0)^{1/2}\psi_0\|_{L^2}^2 .$$

Consequence 2 : the nonlinearity induces a “loss of derivative” :

instead of $\|G(u)\|_{B^1} \le C\,\|u\|^3_{B^1}$, one has $\|G(u)\|_{B^1} \le C\,\|u\|^3_{B^2}$.

$\Longrightarrow$ Lack of estimate.

Alternative proof : take advantage of the energy estimate for well-prepared initial data, polarized on the first eigenmode of $\mathcal{H}_z$.

By combining the equations of conservation of the charge and of conservation of the energy, one gets

$$\|\nabla_x \psi^\varepsilon(t)\|^2_{L^2} + \frac{1}{|\log\varepsilon|}\left\|V^\varepsilon(t)|\psi^\varepsilon(t)|^2\right\|_{L^1} + \frac{1}{\varepsilon^2}\|(\mathcal{H}_z - E_0)^{1/2}\psi^\varepsilon(t)\|^2_{L^2}$$

$$= \|\partial_x \psi_0\|^2_{L^2} + \frac{1}{|\log\varepsilon|}\left\|V^\varepsilon(0)|\psi_0|^2\right\|_{L^1} \qquad \le C\,.$$

Theorem. *Let* $\psi_0(x,z) = \phi_0(x)\chi_0(z)$ *with* $\phi_0 \in H^1(\mathbb{R})$.

Then, as $\varepsilon \longrightarrow 0$*, the filtered function* ϕ^ε *converges locally uniformly in time in the* B^s *topology, for all* $s \in [0,1)$*, to the function* $\phi(t,x)\chi_0(z)$*, where* ϕ *solves the system*

$$i\partial_t \phi = -\partial_x^2 \phi + \frac{1}{2\pi}|\phi|^2 \phi \,, \qquad \phi(t=0) = \phi_0 \,.$$

Remark that the Poisson nonlinearity becomes a cubic local nonlinearity at the limit.

5. Conclusion and extensions

- At least in the cases studied here, no interaction between the fast oscillations $e^{it\mathcal{H}_z/\varepsilon^2}$ and the Poisson nonlinearity.
- This situation is different with the case of the NLS equation with a cubic nonlinearity (see talk of F. Castella), where resonant terms remain at the limit.
- The reason here is that V is independent of z at the limit.

- At least in the cases studied here, no interaction between the fast oscillations $e^{it\mathcal{H}_z/\varepsilon^2}$ and the Poisson nonlinearity.
- This situation is different with the case of the NLS equation with a cubic nonlinearity (see talk of F. Castella), where resonant terms remain at the limit.
- The reason here is that V is independent of z at the limit.

Extensions (in progress...)

- 1DEG, case with general initial data in the energy space.
- 2DEG and 1DEG on bounded domains : towards a numerical approximation of the Poisson equation.
- 2DEG with a strong magnetic field.