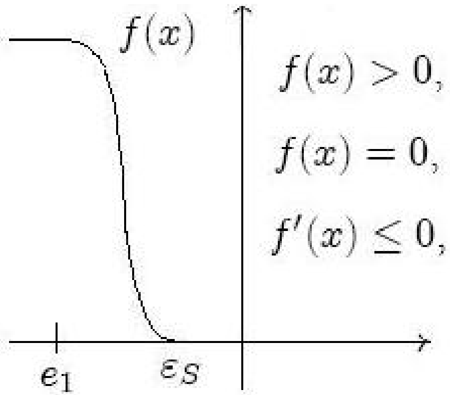
Double scale analysis of a Schrödinger-Poisson system with quantum wells and macroscopic nonlinearities in dimensions 2 and 3.*

*In collaboration with F. Nier and A. Faraj

The model

$U \in C_0^\infty(\mathbb{R}^d)$, Potential well supported inside the sphere of radius h and center $\underline{x}_0$ $\longrightarrow U^h(x) = U\left(\frac{x - x_0}{h}\right)$

$$\begin{cases} \left[-h^2\Delta + U^h + V^h\right]\Psi_i^h = \varepsilon_i^h \Psi_i^h & \text{in } \Omega \\ -\Delta V^h = \sum_{i\subset\mathbb{N}} f(\varepsilon_i^h)|\Psi_i^h|^2 & \text{in } \Omega \\ \Psi_i^h\big|_{\partial\Omega} = 0, \quad V^h\big|_{\partial\Omega} = 0 \end{cases}$$



$f(x) > 0, \quad \forall x < \varepsilon_S$

$f(x) = 0, \quad \forall x \geq \varepsilon_S$

$f'(x) \leq 0, \quad \forall x \in \mathbb{R}$

Changing scale: $\tilde{\Psi}^h(x) = h^{\frac{3}{2}}\Psi^h(hx + x_0), \quad x \in \Omega^h = \left\{x \in \mathbb{R}^3 \,|\, hx + x_0 \in \Omega\right\}$

$$\boxed{\begin{cases} \left(-\Delta + U + \tilde{V}^h\right)\tilde{\Psi}_i^h = \varepsilon_i^h \tilde{\Psi}_i^h & \text{en } \Omega^h \\ -\Delta \tilde{V}^h = h^{d-2}\sum_{i\in\mathbb{N}} f(\varepsilon_i^h)|\tilde{\Psi}_i^h|^2 & \text{en } \Omega^h \\ \tilde{V}^h\big|_{\partial\Omega^h} = 0\,, \quad \tilde{\Psi}_i^h\big|_{\partial\Omega^h} = 0 \end{cases}}$$

$\longrightarrow$ *quantum scale*

Hyp: $e_1 := \inf \sigma\left(-\Delta|_{\mathbb{R}^d} + U\right) < \varepsilon_S$

Spectral asymptotics as $h \to 0$

1. *Agmon estimates for* $\varepsilon_i^h \leq \varepsilon < 0$:

$$\begin{cases} \left\| h\,\nabla \left(e^{c_0|\cdot - x_0|/h} \Psi_i^h \right) \right\|_{L^2(\Omega)} + \left\| e^{c_0|\cdot - x_0|/h} \Psi_i^h \right\|_{L^2(\Omega)} \leq C_0 \\ \left\| e^{c_0|\cdot|}\, \tilde{\Psi}_i^h \right\|_{L^2(\Omega^h)} + \left\| e^{c_0|\cdot|}\, \nabla \tilde{\Psi}_i^h \right\|_{L^2(\Omega^h)} \leq C_1 \\ \left\| e^{c_0|\cdot|}\, \tilde{\Psi}_i^h \right\|_{L^p(\Omega^h)} \leq C_2, \quad p < 6 \end{cases}$$

2. *Spectral convergence:* $\inf \sigma \left(- \Delta|_{\Omega^h} + U \right) \xrightarrow[h \to 0]{} \inf \sigma \left(- \Delta|_{\mathbb{R}^d} + U \right) = e_1 < \varepsilon_S$

- Note: if $\varepsilon_1^h \geq \varepsilon_S \Longrightarrow \begin{cases} \tilde{V}^h = 0 \\ \varepsilon_1^h = \inf \sigma \left(- \Delta|_{\Omega^h} + U \right) \end{cases}$

The hypothesis: $e_1 := \inf \sigma \left(- \Delta|_{\mathbb{R}^d} + U \right) < \varepsilon_S$ and the nonlinearity of the problem give an asymptotic bound for the first energy level:

$$\boxed{\varepsilon_1^h < \varepsilon_S} \quad \forall h \in (0, h_0]$$

3. *Apriori estimate on the charge density (Nier 1993)* : $\left\| \sum_{i\in\mathbb{N}} f(\varepsilon_i^h)|\Psi_i^h|^2 \right\|_{H^{-1}(\Omega)} \leq C$ unif. w.r.t. h

4. *Distributional convergence* : $1_{\varepsilon_i^h \leq \varepsilon < 0} |\Psi_i^h|^2 \to \delta(\cdot - x_0)$

- As a consequence of (3) and (4),

$$\lim_{h\to 0} f(\varepsilon_i^h) = 0 \quad \forall \varepsilon_i^h$$

Lemma 1 *Under the assumption* $\inf \sigma\left(-\Delta|_{\mathbb{R}^d} + U\right) < \varepsilon_S$, *we have:*

$$\lim_{h\to 0} \varepsilon_1^h = \varepsilon_S$$

$$\liminf_{h\to 0} \varepsilon_i^h \geq \varepsilon_S \qquad i > 1$$

Asymptotic estimates at the quantum scale

With the notation $A_i^h = h^{2-d} f(\varepsilon_i^h)$:

$$\begin{cases} \left(-\Delta + U + \tilde{V}^h\right)\tilde{\Psi}_i^h = \varepsilon_i^h \tilde{\Psi}_i^h, & \text{in } \Omega^h \\ -\Delta \tilde{V}^h = \sum_{i\le N_0} A_i^h \left|\tilde{\Psi}_i^h\right|^2, & \text{in } \Omega^h \\ \tilde{V}^h\Big|_{\partial\Omega^h} = 0\,, \quad \tilde{\Psi}_i^h\Big|_{\partial\Omega^h} = 0 \end{cases}$$

Lemma 2 *The coefficients* $A_{i\le N_0}^h$ *show the following properties:*
· *In dimension* $d = 3$*: the set* $\left\{A_{i\le N_0}^h, h\in (0,h_0]\right\}$ *is uniformly bounded w.r.t.* h.
· *In dimension* $d = 2$*: the set* $\left\{\ln \frac{1}{h} A_{i\le N_0}^h, h\in (0,h_0]\right\}$ *is uniformly bounded w.r.t.* h.
where $(0,h_0]$ *is a suitable right neighbourhood of the origin.*

Sketch of the proof*:* $\varepsilon_S > \varepsilon_1^h \ge \left(\inf_{x\in B_r} \tilde{V}^h\right)\int_{B_r} |\tilde{\Psi}_i^h|^2 dx \ge \frac{1}{2}\inf_{x\in B_r}\tilde{V}^h$

$$-\Delta_{\Omega^h}^D W^h = 1_{B_r}\sum_{i\le N_0} A_i^h |\tilde{\Psi}_i^h(x)|^2, \quad W^h\Big|_{B_r} \ge C_r \sum_{i\le N_0} A_i^h$$

$$-\Delta_{\Omega^h}^D\left(\tilde{V}^h - W^h\right) = \left(1 - 1_{B_r}\right)\sum_{i\le N_0} A_i^h |\tilde{\Psi}_i^h(x)|^2 \longrightarrow \tilde{V}^h \ge W^h \text{ in } \Omega^h$$

Lemma 3 *For $i \leq N_0$, $\varepsilon \in (-\|U\|_{L^\infty}, 0)$ and $h \in (0, h_0]$, with $h_0 > 0$ small enough, the following properties hold:*

· *In dimension $d = 3$, the family $\left(1_{\Omega^h} 1_{\varepsilon_i^h < \varepsilon} \tilde{\Psi}_i^h\right)_{h \in (0, h_0]}$ is relatively compact in $L^p(R^3)$ with $p \in [1, 6)$.*

· *In dimension $d = 2$, the family $\left(1_{\Omega^h} 1_{\varepsilon_i^h < \varepsilon} \tilde{\Psi}_i^h\right)_{h \in (0, h_0]}$ is relatively compact in $L^p(R^2)$ with $p \in [1, +\infty)$.*

· *Hence in both cases $\left(\left|1_{\Omega^h} 1_{\varepsilon_i^h < \varepsilon} \tilde{\Psi}_i^h\right|^2\right)_{h \in (0, h_0]}$ is relatively compact in $L^1 \cap L^2(R^d)$.*

Sketch of the proof: $\left\|1_{\Omega^h} 1_{\varepsilon_i^h < \varepsilon} \tilde{\Psi}_i^h\right\|_{L^p(R^d)} \leq C, \quad \forall h \in (0, h_0]$

For any bounded domain $B \subset R^d$

$$\left\|1_{\Omega^h} 1_{\varepsilon_i^h < \varepsilon} \tilde{\Psi}_i^h\right\|_{H^1(B)} \leq \left\|\tilde{\Psi}_i^h\right\|_{H^1(\Omega^h)} \leq \left\|e^{c_0|\cdot|} \nabla \tilde{\Psi}_i^h\right\|_{L^2(\Omega^h)} + \left\|e^{c_0|\cdot|} \tilde{\Psi}_i^h\right\|_{L^2(\Omega^h)} \leq C$$

$$\left\|1_{\Omega^h} 1_{\varepsilon_i^h < \varepsilon} \tilde{\Psi}_i^h\right\|_{L^p(\mathbb{R}^d \setminus B)}^p \leq \sup_{x \in \mathbb{R}^d \setminus B} e^{-p\, c_0 |x|} \left(\int_{\Omega^h} \left|e^{c_0|x|} \tilde{\Psi}_i^h\right|^p dx\right) \leq C' \sup_{x \in \mathbb{R}^d \setminus B} e^{-p\, c_0|x|}$$

Theorem 1 (The 3-D case**)** *Let* $d = 3$ *and let* V^h *(resp.* $\tilde{V}^h$*) solve the Schrodinger-Poisson problem at the classical (resp. quantum) scale.*

· *The potential at the classical scale,* V^h*, converges strongly to* 0 *in* $H_0^1(\Omega)$

$$\left\|V^h\right\|_{H_0^1(\Omega)} = \mathcal{O}(h^{1/2})$$

· *By fixing the threshold* ε_S *associated with* f*, there exists a unique* $(A, W) \in (0, +\infty) \times \dot{H}^1(R^3; R)$ *such that* $\varepsilon_S = \inf \sigma(-\Delta + U + W)$ *and*

$$\begin{cases} [-\Delta + U + W]\, \chi = \varepsilon_S\, \chi\,, \quad \text{with} \quad \chi \in H^2(\mathbb{R}^3),\ \|\chi\|_{L^2(\mathbb{R}^3)} = 1\,, \\ -\Delta W = A\, |\chi|^2\,. \end{cases}$$

· *With above notations, the potential at the quantum scale* $\tilde{V}^h$ *satisfies*

$$\lim_{h \to 0} \left\| 1_{\Omega^h} \tilde{V}^h - W \right\|_{L^\infty(\mathbb{R}^3)} = 0\,.$$

· *There exists* $h_1 > 0$ *such that the eigenvalues* ε_i^h *are larger than* ε_S *and* $f(\varepsilon_i^h) = 0$ *for all* $i \geq 2$ *and all* $h \leq h_1$*. The particle density at the quantum scale,* $h^{-1} \sum_{i \in \mathbb{N}} f(\varepsilon_i^h) |\tilde{\Psi}_i^h|^2 = h^{-1} f(\varepsilon_1^h) \left|\tilde{\Psi}_1^h\right|^2$ *for* $h \leq h_1$*, satisfies*

$$\lim_{h \to 0} \left\| 1_{\Omega^h} h^{-1} f(\varepsilon_1^h) |\tilde{\Psi}_1^h|^2 - A|\chi|^2 \right\|_{L^1 \cap L^2(\mathbb{R}^3)} = 0\,.$$

Strategy of the proof:

1. A consequence of the Lemmas 2 and 3: *out of any infinite subset* $S \subset (0, h_0]$ *with* $0 \in \overline{S}$, *we can extract* $D \subset S$, $0 \in D$, *such that*

$$A_i = \lim_{\substack{h \to 0 \\ h \in D}} A_i^h \geq 0, \quad \lim_{\substack{h \to 0 \\ h \in D}} \left\| 1_{\Omega^h} 1_{\varepsilon_i^h < \varepsilon} \tilde{\Psi}_i^h - \chi_i \right\|_{L^2 \cap L^4(\mathbb{R}^3)} = 0$$

$$\boxed{\lim_{\substack{h \to 0 \\ h \in D}} \left\| 1_{\Omega^h} \sum_{i \leq N_0} A_i^h \left| \tilde{\Psi}_i^h \right|^2 - \rho \right\|_{L^1 \cap L^2(\mathbb{R}^3)} = 0} \quad \text{with } \rho = \sum_{i \leq N_0} A_i \left| \chi_i \right|^2 \qquad \text{(II)}$$

Let G be the Green function of $-\Delta$ and assume $f \in L^1 \cap L^2(\mathbb{R}^3)$

$$\to \begin{cases} G * f \in C_\infty(\mathbb{R}^3) \\ \|G * f\|_{L^\infty(\mathbb{R}^3)} \leq C \left(\|f\|_{L^1(\mathbb{R}^3)} + \|f\|_{L^2(\mathbb{R}^3)} \right) \end{cases}$$

Under the assumptions (I) and (II), and: $-\Delta_{\Omega^h}^D \tilde{V}^h = \sum_{i \leq N_0} A_i^h \left| \tilde{\Psi}_i^h \right|^2$

$$\left\| \tilde{V}^h - G * \rho \right\|_{L^\infty(\Omega^h)} \leq \sup_{x \in \partial \Omega^h} |G * \rho| + 2 \left\| G * \left(\rho - 1_{\Omega^h} \sum_{i \leq N_0} A_i^h \left| \tilde{\Psi}_i^h \right|^2 \right) \right\|_{L^\infty(\mathbb{R}^3)} \to 0$$

$$\left\| V^h \right\|_{H_0^1(\Omega)} = h^{1/2} \left\| \tilde{V}^h \right\|_{H_0^1(\Omega^h)} \leq h^{\frac{1}{2}} \left\| \tilde{V}^h \right\|_{L^\infty(\mathbb{R}^3)} \sum_{i \leq N_0} A_i^h$$

2. $$N_1 = \max\left\{ i \,\middle|\, \liminf_{h\to 0} \varepsilon_i^h = \varepsilon_S \right\}, \qquad \lim_{\substack{h\to 0\\ h\in D}} \varepsilon_{i\le N_1}^h = \varepsilon_S$$

For $i \le N_1$, $\varphi \in C_0^\infty(\mathbb{R}^3)$

$$\lim_{\substack{h\to 0\\ h\in D}} \left(\left[-\Delta + U + \tilde{V}^h - \varepsilon_i^h \right] \varphi,\, 1_{\Omega^h} \tilde{\Psi}_i^h \right)_{L^2(\mathbb{R}^3)} = \left(\left[-\Delta + U + G * \rho - \varepsilon_S \right] \varphi,\, \chi_i \right)_{L^2(\mathbb{R}^3)}$$

$$\Rightarrow \begin{cases} \left[-\Delta + U + G * \rho \right] \chi_i = \varepsilon_S \, \chi_i \quad \text{in } L^2\left(\mathbb{R}^3\right),\ i = 1, \ldots, N_1 \\ \|\chi_i\|_{L^2(\mathbb{R}^3)} = 1\,, \quad \left(\chi_i, \chi_j\right)_{L^2(\mathbb{R}^3)} = \delta_{ij} \end{cases}$$

For $i = 1$:

$$\tilde{\Psi}_1^h \ge 0 \quad \text{a.e. on } \Omega^h \longrightarrow \chi_1 \ge 0 \quad \text{a.e. in } \mathbb{R}^3$$

· Note: The unique non negative eigenvector coincides with the fundamental mode

$$\Rightarrow \boxed{N_1 = 1} \quad \text{and the limit problem writes as:}$$

$$\begin{cases} \left[-\Delta + U + W \right] \chi = \varepsilon_S \, \chi, \quad \|\chi\|_{L^2(\mathbb{R}^3)} = 1, \\ \varepsilon_S = \inf \sigma \left(-\Delta + U + W \right)\,, \\ -\Delta W = A_1 \, |\chi_1|^2\,. \end{cases}$$

3. We consider the functional $K_a : \dot{H}^1(\mathbb{R}^3;\mathbb{R}) \longrightarrow \mathbb{R}$

$$K_a(W) = \frac{1}{2}\int_{\mathbb{R}^3} (\nabla W)^2 \, dx - a\,\varepsilon(W)\,, \quad a \geq 0$$

$$\varepsilon(W) = \inf \sigma(-\Delta_{\mathbb{R}^3} + U + W), \quad \Big[-\Delta_{\mathbb{R}^3} + U + W\Big]\,\psi(W) = \varepsilon(W)\,\psi(W)$$

· The maps $\varepsilon(W)$, $\psi(W)$ are continuous in $\dot{H}^1(\mathbb{R}^3;\mathbb{R})$ and analytic in the open set

$$S = \Big\{W \in \dot{H}^1(\mathbb{R}^3;\mathbb{R})\,,\ \varepsilon(W) < 0\Big\}$$

The map $K_a(W)$ admits a unique global minimum W_a. If $W_a \in S$

$$\Rightarrow \begin{cases} [-\Delta + U + W_a]\,\psi_a = \varepsilon_a \psi_a \\ -\Delta W_a = a\,|\psi_a|^2 \end{cases} \qquad \text{with } \varepsilon_a = \varepsilon(W_a),\ \psi_a = \psi(W_a)$$

Proposition The map $a \mapsto \varepsilon_a$ is continuous in $\mathbb{R}^+$. Moreover it is analytic and strictly increasing in the domain $a \in \boldsymbol{\Sigma} = \Big\{a \in \mathbb{R}^+ \,|\, \varepsilon_a < 0\Big\}$.

Sketch of the proof: We exploit the convexity of $K_a(W)$ and

$$\varepsilon_a' = d_W^2 K_a(W_a) \cdot (W_a', W_a') \geq 0$$

Theorem 2 (The 2-D case**)** *Let $d = 2$ and let V^h (resp. $\tilde{V}^h$) solve the Schrodinger-Poisson problem at the classical (resp. quantum) scale.*

· *The potential at the classical scale, V^h, converges strongly to 0 in $H_0^1(\Omega)$*

$$\left\|V^h\right\|_{H_0^1(\Omega)} = \mathcal{O}\left(\frac{1}{|\ln h|}\right) .$$

· *Take the threshold ε_S associated with f and $e_1 = \inf\sigma(-\Delta + U)$ and set $\theta = \varepsilon_S - e_1$. Then the potential $\tilde{V}^h$ at the quantum scale satisfies for any fixed $\kappa > 0$:*

$$\lim_{h\to 0}\left\|\tilde{V}^h - \theta\right\|_{L^\infty(\{|x|\leq -\kappa\ln h\})} = 0$$

· *There exists $h_1 > 0$ such that the eigenvalues ε_i^h are larger than ε_S and $f(\varepsilon_i^h) = 0$ for all $i \geq 2$ and all $h \leq h_1$. The particle density at the quantum scale, $\sum_{i\in\mathbb{N}} f(\varepsilon_i^h)|\tilde{\Psi}_i^h|^2 = f(\varepsilon_1^h)\left|\tilde{\Psi}_1^h\right|^2$ for $h \leq h_1$, satisfies*

$$\left\|1_{\Omega^h} f(\varepsilon_1^h)\left|\tilde{\Psi}_1^h\right|^2\right\|_{L^2(\mathbb{R}^2)} = \mathcal{O}(|\ln h|^{-1}) ,$$

$$\lim_{h\to 0}|\ln h|\left\|1_{\Omega^h} f(\varepsilon_1^h)\left|\tilde{\Psi}_1^h\right|^2\right\|_{L^1(\mathbb{R}^2)} = \lim_{h\to 0}|\ln h|\, f(\varepsilon_1^h) = 2\pi\theta .$$

Strategy of the proof: Let us introduce the rescaled density r^h

$$B_i^h = |\ln h|\ A_i^h, \quad r^h = \sum_{i \le N_0} B_i^h \left|\tilde{\Psi}_i^h\right|^2$$

Out of any $S \subset (0, h_0]$, $0 \in \bar{S}$, we can extract a subset $D \subset S$, $0 \in \bar{D}$, such that

$$\lim_{\substack{h \to 0 \\ h \in D}} B_i^h = B_i, \quad \lim_{\substack{h \to 0 \\ h \in D}} \left\| 1_{\Omega^h} r^h - r \right\|_{L^1 \cap L^2(\mathbb{R}^2)} \tag{III}$$

$$\boxed{\sum_{i \le N_0} A_i^h \left|\tilde{\Psi}_i^h\right|^2 = |\ln h|^{-1} r^h} \Longrightarrow \left\| \sum_{i \le N_0} A_i^h \left|\tilde{\Psi}_i^h\right|^2 \right\|_{L^1 \cap L^2(\Omega^h)} = \mathcal{O}(|\ln h|^{-1})$$

· Our strategy consistes into a direct estimate of the L^∞-norm of $\tilde{V}^h$ in regions of size $\mathcal{O}(|\ln h|)$. Let $R^h = \kappa\,(|\ln h|)$ with $\kappa > 0$. Under the assumption (III), we prove that

$$\lim_{\substack{h \to 0 \\ h \in D}} \left\| \tilde{V}^h - \theta \right\|_{L^\infty(B_{R^h})} = 0, \qquad \theta = \frac{1}{2\pi} \sum_{i \le N_0} B_i$$

$$\left\| \tilde{V}^h \right\|_{L^\infty(\mathbb{R}^2 \setminus B_{R^h})} \le C \quad \text{and} \quad \left\| V^h \right\|_{H_0^1(\Omega)} = \mathcal{O}\left(\frac{1}{|\ln h|}\right) \quad \forall h \in D$$

· Next, using Agmon estimates and the standard inequality:

$$||u||_{L^2(\mathbb{R}^2)} d(\lambda, \sigma(H)) \leq ||(H-\lambda)u||_{L^2(\mathbb{R}^2)}$$

we prove:

$$\inf \sigma(-\Delta_{\Omega^h} + U + \tilde{V}^h) \underset{h \to 0}{\longrightarrow} \inf \sigma(-\Delta_{\mathbb{R}^2} + U + \theta) = e_1 + \theta$$

$$\Longrightarrow \begin{cases} \lim\limits_{h\to 0} \varepsilon_1^h = e_1 + \theta \\ \lim\limits_{h\to 0} \inf \varepsilon_i^h > \varepsilon_S \quad \text{for } i > 1 \end{cases}$$

Then: $\boxed{\theta = \varepsilon_S - e_1}$ and

$$2\pi\theta = \sum_{i \leq N_0} B_i = \lim_{h \to 0} |\ln h| \left\| 1_{\Omega^h} f(\varepsilon_1^h) \left| \tilde{\Psi}_1^h \right|^2 \right\|_{L^1(\mathbb{R}^2)}$$