

Effective quantum Hamiltonian in thin domains with non-homogeneity

Romana Kvasničková

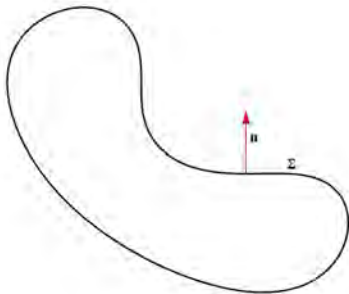
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Faculty of Nuclear Sciences and Physical Engineering

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Based on: R. K., arXiv:2204.11709 (2022), to appear in Differ. Integral. Equ.

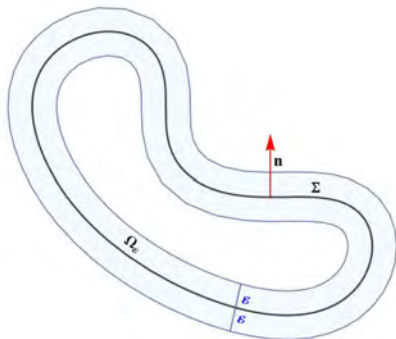
Motivation: homogeneous case

M. Schatzman, Applicable Anal. (1996)



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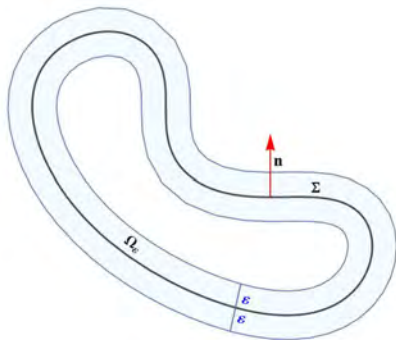
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- the spectral problem

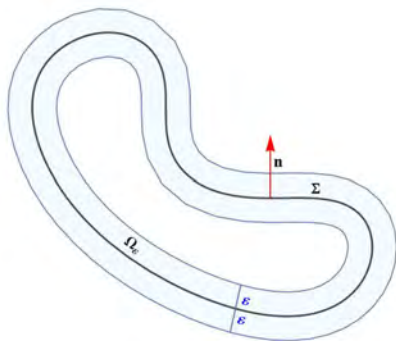
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$$a(x) = 1 \text{ in } \Omega_\varepsilon$$

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Result

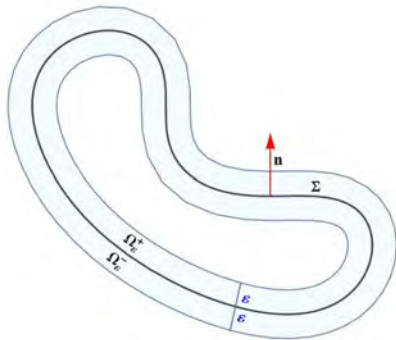
$$(\lambda_\varepsilon)_k = \lambda_k + O(\varepsilon) \quad \text{as } \varepsilon \rightarrow 0, \quad \{\lambda_k\}_{k=0}^\infty = \sigma(-\Delta^\Sigma)$$

Motivation: “Yachimura’s problem”



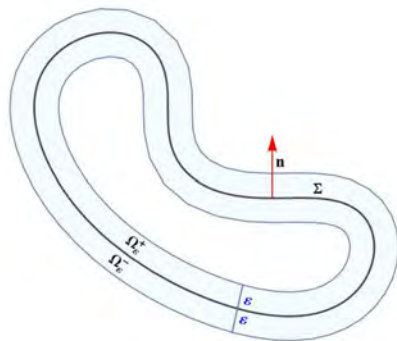
T. Yachimura, Differ. Integral. Equ. (2018)

- $\Omega_\varepsilon = \Omega_\varepsilon^- \cup \Omega_\varepsilon^+ \cup \Sigma$



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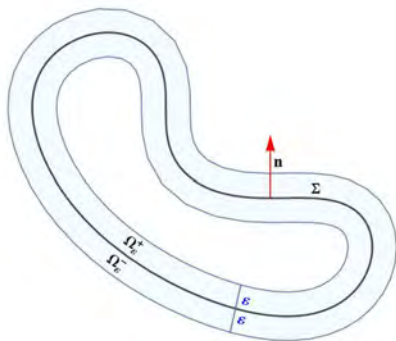
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Result

$$(\lambda_\epsilon)_k = \frac{a_- + a_+}{2} \lambda_k + O(\epsilon) \quad \text{as } \epsilon \rightarrow 0, \quad \{\lambda_k\}_{k=0}^\infty = \sigma(-\Delta^\Sigma)$$

Our goals and strategy

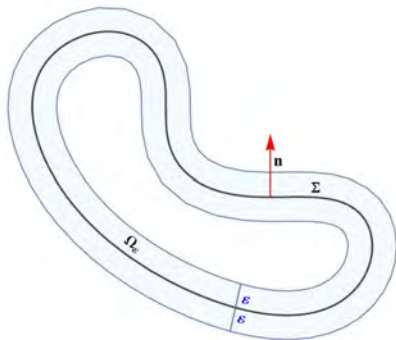
- Goals
 - insight into the result
 - more general models
 - more general results of the convergence
 - the rate of the convergence

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- Goals
 - insight into the result
 - more general models
 - more general results of the convergence
 - the rate of the convergence
- Strategy
 - interpretation of the operator as the quantum Hamiltonian

Analytical generalization

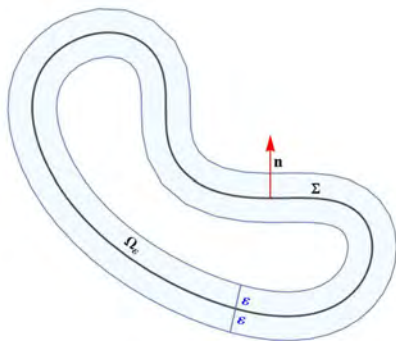
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- construction of Ω_ε

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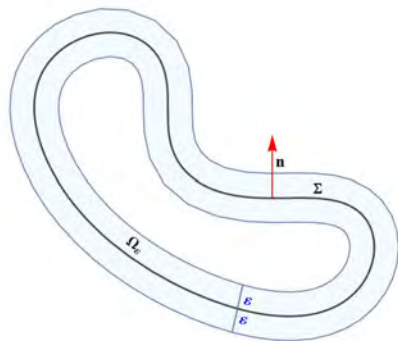


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$$\begin{cases} -\nabla \cdot a \nabla \tilde{v}_\varepsilon = \lambda_\varepsilon \tilde{v}_\varepsilon & \text{in } \Omega_\varepsilon \\ \frac{\partial \tilde{v}_\varepsilon}{\partial \tilde{n}} = 0 & \text{on } \partial\Omega_\varepsilon \end{cases}$$

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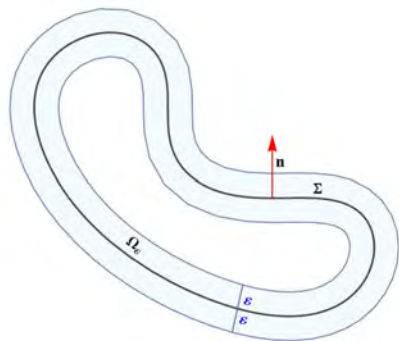
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- the operator \tilde{H}_ϵ on $L^2(\Omega_\epsilon)$

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- the operator \tilde{H}_ϵ on $L^2(\Omega_\epsilon)$

- demands on the function $a : \Omega_\epsilon \rightarrow \mathbb{R}^+$

$$(\exists C > 0) (\forall \epsilon \in (0, 1)) (\text{almost every } x \in \Omega_\epsilon) \left(\frac{1}{C} \leq a(x) \leq C \right)$$

Physical interpretation

- interpretation of the operator \tilde{H}_ε on $L^2(\Omega_\varepsilon)$ as the quantum Hamiltonian of a (quasi)particle in a non-homogeneous nanostructure

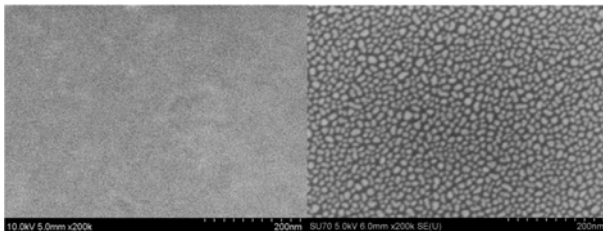


Figure: silicon nanostructured semiconductor

Physical interpretation

- interpretation of the operator \tilde{H}_ϵ on $L^2(\Omega_\epsilon)$ as the quantum Hamiltonian of a (quasi)particle in a non-homogeneous nanostructure
- correspondce of the equation

$$\tilde{H}_\epsilon \tilde{v}_\epsilon = \lambda_\epsilon \tilde{v}_\epsilon$$

with the stationary Schrödinger equation

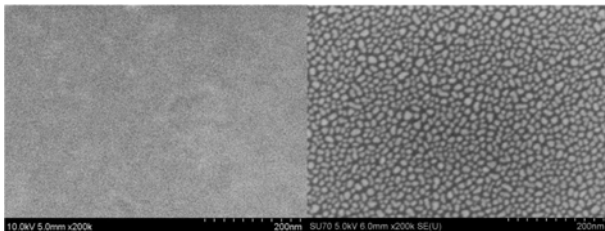


Figure: silicon nanostructured semiconductor

Strategy: transformation

D. Krejčířík, N. Raymond, M. Tušek, J. Geom. Anal. (2015)

- transformation between Ω_ε and $\Omega \equiv \Sigma \times (-1, 1)$

$$\mathcal{L}_\varepsilon : \Omega \longrightarrow \Omega_\varepsilon : \{(s, t) \mapsto s + \varepsilon t \vec{n}\}$$

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- unitary transformation

$$U : L^2(\Omega_\varepsilon) \longrightarrow L^2(\Omega, f_\varepsilon(s, t) \, d\Sigma \wedge dt) : \{\tilde{v} \mapsto v = \sqrt{\varepsilon} \tilde{v} \circ \mathcal{L}_\varepsilon\}$$

$$\varepsilon f_\varepsilon = |G_\varepsilon|^{1/2} |g|^{-1/2}$$

$$a_\varepsilon = a \circ \mathcal{L}_\varepsilon$$

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$$\varepsilon f_\varepsilon = |G_\varepsilon|^{1/2} |g|^{-1/2} \qquad a_\varepsilon = a \circ \mathcal{L}_\varepsilon$$

- the operator $H_\varepsilon \equiv U \tilde{H}_\varepsilon U^{-1}$ on $L^2(\Omega, f_\varepsilon(s, t) d\Sigma \wedge dt)$

$$Q_\varepsilon[v] = \int_\Omega a_\varepsilon \left[\left(\frac{\partial \bar{v}}{\partial s^\mu} G_\varepsilon^{\mu\nu} \frac{\partial v}{\partial s^\nu} \right) + \frac{1}{\varepsilon^2} \left| \frac{\partial v}{\partial t} \right|^2 \right] f_\varepsilon d\Sigma \wedge dt$$

$$D(Q_\varepsilon) = W^{1,2}(\Omega, f_\varepsilon(s, t) d\Sigma \wedge dt)$$

Effective model

- the operator \tilde{H}_{eff} on $L^2(\Sigma, d\Sigma)$

$$\lambda_{\text{eff}} \in \sigma(\tilde{H}_{\text{eff}}) \longleftrightarrow -|g|^{-\frac{1}{2}} \frac{\partial}{\partial s^\mu} \left(|g|^{\frac{1}{2}} \bar{a} g^{\mu\nu} \frac{\partial \varphi_{\text{eff}}}{\partial s^\nu} \right) = \lambda_{\text{eff}} \varphi_{\text{eff}} \quad \text{in } \Sigma$$

$$\bar{a}(s) = \lim_{\varepsilon \rightarrow 0} \frac{1}{2} \int_{-1}^1 (a_\varepsilon f_\varepsilon)(s, t) dt$$

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$$a_\varepsilon(s, t) = \begin{cases} a_+ & t \in (0, 1) \\ a_- & t \in (-1, 0) \end{cases}$$

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- convergence to the effective model

$$“H_\varepsilon \xrightarrow[\varepsilon \mapsto 0]{?} \tilde{H}_{\text{eff}}”$$

Resolvent convergence

Definition

Let A and A_k be self-adjoint operators on a Hilbert space \mathcal{H} for any $k \in \mathbb{N}$. Then $\{A_k\}_{k=1}^{\infty}$ is said to converge to A in the **norm-resolvent** sense if

$$\lim_{k \rightarrow \infty} \|R_k(z) - R(z)\|_{\mathcal{H} \rightarrow \mathcal{H}} = 0$$

for all $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$. R_k and R are resolvent operators of A_k and A .

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- extension of the action H_{eff} of the operator \tilde{H}_{eff} on $\mathcal{H}_0 := \{\varphi \otimes \chi_0 \mid \varphi \in L^2(\Sigma)\} \subset L^2(\Omega, d\Sigma \wedge dt)$

$$H_{\text{eff}} := \pi^{-1} \tilde{H}_{\text{eff}} \pi \quad \pi : \mathcal{H}_0 \rightarrow L^2(\Sigma) : \{\varphi \otimes \chi_0 \rightarrow \varphi\}$$

The Rate of Norm-Resolvent Convergence

$$\langle a_\varepsilon \rangle(s) = \frac{1}{2} \int_{-1}^1 (a_\varepsilon f_\varepsilon)(s, t) dt \quad \bar{a}(s) = \lim_{\varepsilon \rightarrow 0} \langle a_\varepsilon \rangle(s)$$

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Theorem

Let a_ε be a positive function satisfying:

- 1 $(\exists C > 0) (\forall \varepsilon \in (0, 1))$ (almost every $(s, t) \in \Sigma \times (-1, 1)$)
$$\left(\frac{1}{C} \leq a_\varepsilon(s, t) \leq C \wedge |\nabla_g a_\varepsilon|_g \leq C \right),$$
- 2 $(\forall s \in \Sigma) \left(\langle a_\varepsilon \rangle \xrightarrow{\varepsilon \rightarrow 0} \bar{a} \right),$
- 3 $d(\varepsilon) := \|\langle a_\varepsilon \rangle - 2\bar{a}\|_{L^\infty(\Sigma)} \xrightarrow{\varepsilon \rightarrow 0} 0.$

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Then there exists a positive constant C such that

$$\left\| U_\varepsilon (H_\varepsilon + 1)^{-1} U_\varepsilon^{-1} - (H_{\text{eff}} + 1)^{-1} \oplus 0^\perp \right\| \leq C \max \{ \varepsilon, d(\varepsilon) \}$$

for all sufficiently small ε .

Idea of the proof

- the orthogonal projection

$$P_0 : L^2(\Omega) \rightarrow \mathcal{H}_0 : \left\{ \psi \mapsto \left(\int_{-1}^1 \psi(\cdot, t) \, dt \right) \otimes \chi_0 \right\} \quad P_0^\perp := 1 - P_0$$

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- the definition of $\{\psi_\varepsilon\}_{\varepsilon>0} \in L^2(\Omega, f_\varepsilon \, d\Sigma \wedge dt)$ and $\psi \in \mathcal{H}_0$

$$(H_\varepsilon + 1) \psi_\varepsilon = U_\varepsilon^{-1} G \quad (H_{\text{eff}} + 1) \psi = P_0 F$$

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$$\begin{aligned} & \left(F, \left(U_\varepsilon (H_\varepsilon + 1)^{-1} U_\varepsilon^{-1} - (H_{\text{eff}} + 1)^{-1} \oplus 0^\perp \right) G \right) \\ &= (F, U_\varepsilon (H_\varepsilon + 1)^{-1} U_\varepsilon^{-1} G) - \left(\left((H_{\text{eff}} + 1)^{-1} \oplus 0^\perp \right) F, G \right) \\ &= \left(\left(P_0 + P_0^\perp \right) F, \left(P_0 + P_0^\perp \right) U_\varepsilon \psi_\varepsilon \right) - \left((H_{\text{eff}} + 1)^{-1} P_0 F, G \right) \\ &= \left((H_{\text{eff}} + 1) \psi, P_0 (U_\varepsilon \psi_\varepsilon) \right) + \left(P_0^\perp F, P_0^\perp (U_\varepsilon \psi_\varepsilon) \right) - (\psi, U_\varepsilon (H_\varepsilon + 1) \psi_\varepsilon) \\ &= (H_{\text{eff}} \psi, P_0 (U_\varepsilon \psi_\varepsilon)) + \left(P_0^\perp F, P_0^\perp (U_\varepsilon \psi_\varepsilon) \right) - (U_\varepsilon^{-1} \psi, H_\varepsilon \psi_\varepsilon)_\varepsilon \\ &= h_{\text{eff}}(\psi, P_0 (U_\varepsilon \psi_\varepsilon)) - h_\varepsilon(U_\varepsilon^{-1} \psi, \psi_\varepsilon) + \left(P_0^\perp F, P_0^\perp (U_\varepsilon \psi_\varepsilon) \right) \end{aligned}$$

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$$|h_{\text{eff}}(\psi, P_0(U_\varepsilon \psi_\varepsilon)) - h_\varepsilon(U_\varepsilon^{-1} \psi, \psi_\varepsilon)| \stackrel{?}{\leq} C \max\{\varepsilon, d(\varepsilon)\}$$

Alternative sufficient conditions

- modification of conditions of the convergence

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Conclusions and open problems

- the more general model
- “ $-\operatorname{div} a \operatorname{grad} \xrightarrow{\varepsilon \rightarrow 0} -\operatorname{div}_g \bar{a} \operatorname{grad}_g$ ” in the norm-resolvent sense
- the rate of the convergence
- the decay rate of eigenvalues and eigenfunctions

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Open problems

- optimality of the rate of the convergence
- complex non-homogeneity a