Effective quantum Hamiltonian in thin domains with non-homogeneity

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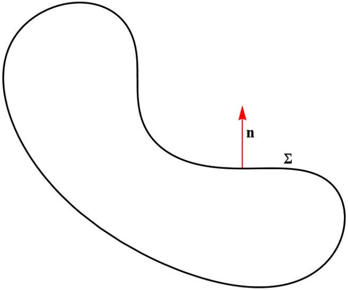
Based on: R. K., arXiv:2204.11709 (2022), to appear in Differ. Integral. Equ.

Motivation: homogeneous case

M. Schatzman, Applicable Anal. (1996)



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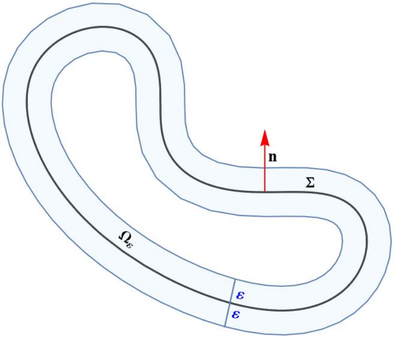

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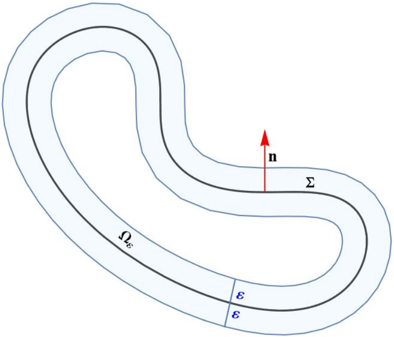

- the spectral problem

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

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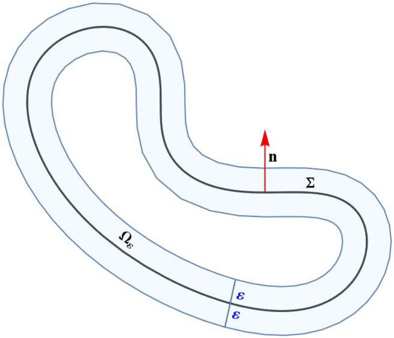

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Result

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

Motivation: "Yachimura's problem"

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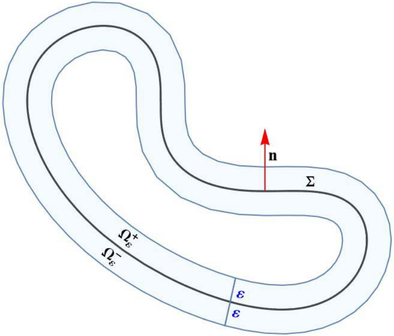

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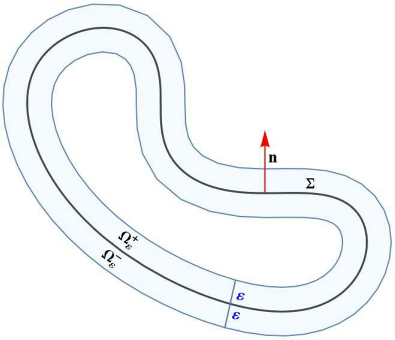

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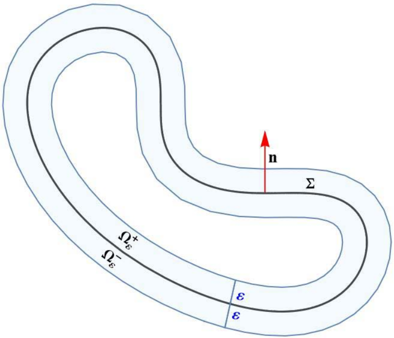

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Result

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

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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- Strategy
  - interpretation of the operator as the quantum Hamiltonian

Analytical generalization

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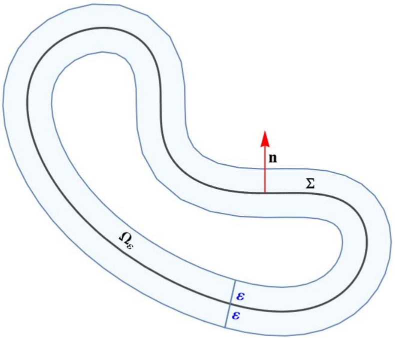

- construction of Ω_ε

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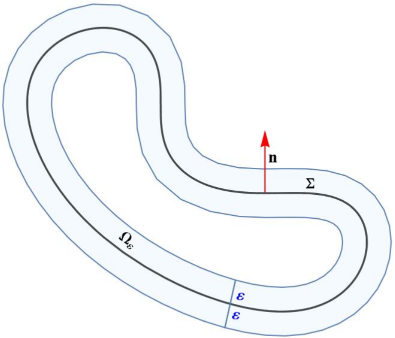

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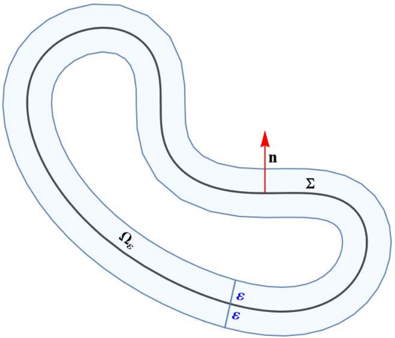

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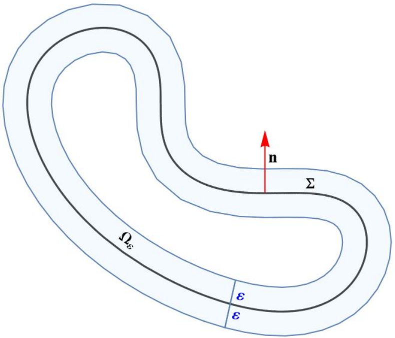

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- the operator $\tilde{H}_\varepsilon$ on $L^2(\Omega_\varepsilon)$

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

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

Physical interpretation

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

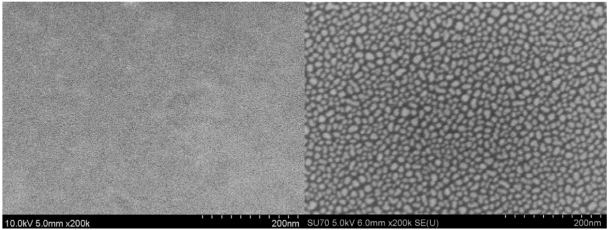

Figure: silicon nanostructured semiconductor

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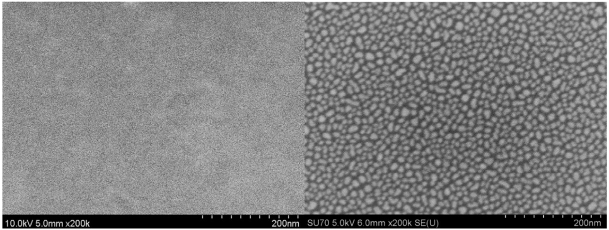
- interpretation of the operator $\tilde{H}_\varepsilon$ on $L^2(\Omega_\varepsilon)$ as the quantum Hamiltonian of a (quasi)particle in a non-homogeneous nanostructure
- correspondce of the equation

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

with the stationary Schrödinger equation



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Strategy: transformation

D. Krejčiřík, 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

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

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

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

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

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

Effective model

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

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

$$\overline{a}(s) = \lim_{\varepsilon \mapsto 0} \frac{1}{2} \int_{-1}^{1} (a_\varepsilon f_\varepsilon)(s,t)\mathrm{d}t$$

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- convergence to the effective model

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

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

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

for all $z \in \mathbb{C}$ with $\mathrm{Im}\, z \neq 0$. 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 $\tilde{H}_{\mathrm{eff}}$ on $\mathcal{H}_0 := \{\varphi \otimes \chi_0 \mid \varphi \in L^2(\Sigma)\} \subset L^2(\Omega, \mathrm{d}\Sigma \wedge \mathrm{d}t)$

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

The Rate of Norm-Resolvent Convergence

$$\langle a_\varepsilon \rangle (s) = \frac{1}{2} \int_{-1}^{1} (a_\varepsilon f_\varepsilon)(s,t)\mathrm{d}t \qquad \overline{a}(s) = \lim_{\varepsilon \mapsto 0} \langle a_\varepsilon \rangle (s)$$

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Theorem

Let a_ε be a positive function satisfying:

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

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Then there exists a positive constant C such that

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

for all sufficiently small ε.

Idea of the proof

- the orthogonal projection

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

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

$$\left(H_\varepsilon + 1\right) \psi_\varepsilon = U_\varepsilon^{-1} G \qquad \left(H_{\mathrm{eff}} + 1\right) \psi = P_0 F$$

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

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

$$|h_{\mathrm{eff}}\left(\psi, P_0(U_\varepsilon \psi_\varepsilon)\right) - h_\varepsilon\left(U_\varepsilon^{-1}\psi, \psi_\varepsilon\right)| \overset{?}{\leq} C \max\{\varepsilon, d(\varepsilon)\}$$

Alternative sufficient conditions

- modification of conditions of the convergence
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  $$\left(\tfrac{1}{C} \leq a_\varepsilon(s,t) \leq C \ \wedge \ \left|\nabla_g a_\varepsilon\right|_g \leq C \right)$$
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  - $d(\varepsilon) = \mathcal{O}(\varepsilon)$ as $\varepsilon \mapsto 0$

Conclusions and open problems

- the more general model
- "$-\mathrm{div}\; a\; \mathrm{grad} \underset{\varepsilon\to 0}{\longrightarrow} -\mathrm{div}_g\; \bar{a}\; \mathrm{grad}_g$" 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