Magnetic bottles for the Neumann problem: curvature effects in the case of dimension 3

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Abstract

In [HeMo3], we have analyzed the recent results obtained on the Neumann realization of the Schrödinger operator in the case of dimension 3 by Lu and Pan. After presenting a short treatment of their spectral analysis of key-models, we show briefly how to implement the techniques of Helffer-Morame in order to give some localization of the ground state. This leaves open the question of the localization by curvature effect which was conjectured by Bernoff-Sternberg in the case of dimension 2 and solved by [LuPa2], [PiFeSt] and [HeMo2]. We shall now analyze the curvature effects in the case of dimension 3.

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1 Introduction

Motivated by the superconductivity[1] (see [He3] or [LuPa4] for a review on this aspect), we would like to analyze the groundstate energy (that is the lowest eigenvalue) of the Neumann realization of the Schrödinger operator with magnetic potential in an open set Ω in $\mathbb{R}^3$, which will be assumed in all the paper to be smooth up to the boundary :

$$P_A^h = \sum_{j=1}^{3} (hD_{x_j} - A_j(x))^2 \ , \tag{1.1}$$

where $A = (A_1, A_2, A_3)$ is a magnetic potential. This realization will be denoted by $P_{A,\Omega}^{h,N}$ but we will sometimes use shorter notations when there is no ambiguity. If $\lambda(h)$ is the lowest eigenvalue and $u^h(x)$ is a corresponding normalized eigenstate, we would like to discuss the asymptotic of $\lambda(h)$ as $h \to 0$, with the hope to analyze after the localization of u^h. This problem was treated in the case of dimension 2 by Bernoff-Sternberg [BeSt], Lu-Pan [LuPa1, LuPa2, LuPa3], Del Pino-Fellmer-Sternberg [PiFeSt] and Helffer-Morame [HeMo2] in a rather complete way. Later a recent work by Lu-Pan [LuPa5] was starting the analysis of the dimension 3 and this was completed slightly in [HeMo3]. So this paper is the continuation of the programme, with a particular emphasis on the constant magnetic field case.

We start by establishing rough estimates, but sufficiently accurate for determining the effective order of the curvature effect.

Theorem 1.1 .
Let Ω be a bounded open set of $\mathbb{R}^3$ with smooth boundary $\partial\Omega$. Let $P_{A,\Omega}^{h,N}$ be the Neumann operator on $L^2(\Omega)$ associated to the Schrödinger operator with constant magnetic field $(hD - A)^2$ and let us assume that the vector magnetic field $H = \mathrm{curl}\,(A)$ is constant and of intensity equal to b.
If $\lambda(h) = \inf \mathrm{Sp}\,(P_{A,\Omega}^{h,N})$ is the first eigenvalue of $P_{A,\Omega}^{h,N}$, then there exists a constant C_0 such that

$$|\lambda(h) - b\Theta_0 h| \leq C_0 h^{\frac{4}{3}} \ . \tag{1.2}$$

[1] One can find in Chapter 4 of [S-JSaTh] a physical presentation of the problem we are considering. We particularly emphasize on their subsection 4.3 where they analyze (with partially heuristic arguments) the angular dependence of the nucleation field. We will give a mathematical proof of, what they describe for example p. 87 :

" For type II superconductors[2] the above calculation shows that superconductivity is not entirely destroyed for $H_{c_2} < H < H_{c_3}$. A superconducting sheath remains close to the surface parallel to the applied field. Conversely, when the field is decreased below H_{c_3}, a superconducting sheath appears at the surface before superconductivity is restored in the bulk at $H = H_{c_2}$. If the sample is a long cylinder with the applied field parallel to the axis, the sheath will cover all the surface of the cylinder. If it is a sphere, the sheath will be restricted to a small zone near the equatorial plane when H is close to H_{c_3}. When the field is decreased towards H_{c_2} the sheath will progressively extend up to the poles."

We observe that in the case of dimension 2, the corresponding error was in $\mathcal{O}(h^{\frac{3}{2}})$.

We then continue with the analysis of the curvature effects, which are the analog in dimension 3 of the results first conjectured by Bernoff-Sternberg (see [BeSt]) in the case of dimension 2. We establish the corresponding conjecture in the case of dimension 3.

Conjecture 1.2 .
Let $P_{A,\Omega}^{h,N}$ be the Neumann realization on $L^2(\Omega)$ of the magnetic Laplacian $(hD - A)^2$, where $h \in]0,1[$ is a small parameter and A corresponds to constant magnetic field. Under a natural generic assumption (satisfied when Ω is a strictly convex open set in $\mathbb{R}^3$), there exists $\eta > 0$ and $\hat{\gamma}_0$ such that :

$$\inf \ \mathrm{Sp}\ (P_{A,\Omega}^{h,N}) = b\Theta_0 h + \hat{\gamma}_0 b^{\frac{2}{3}} h^{\frac{4}{3}} + \mathcal{O}(h^{\eta+\frac{4}{3}}) \ , \tag{1.3}$$

where $\hat{\gamma}_0$ is a complicate explicitely computable magnetic invariant.

The more precise statements are given in Section 9, once all the terms appearing in the computation of $\hat{\gamma}_0$ have been defined. We will prove in this paper the upper bound part of this conjecture and establish the lower bound in an unfortunately non generic, but geometrically natural case, that we now briefly describe.

It is observed by [LuPa5] and this will be recalled in Section 4, that the ground state u^h is localized (as $h \to 0$) near the boundary $\partial\Omega$ but more precisely on the set :

$$\Gamma = \{ x \in \partial\Omega \mid H \cdot N(x) = 0 \} \ , \tag{1.4}$$

where $N(x)$ is the normal at x to $\partial\Omega$.
It is natural to assume that :

$$\Gamma \text{ is a regular submanifold of } \partial\Omega \ . \tag{1.5}$$

At each point x of Γ, we will associate to H (see Definition 8.6) a notion of normal curvature along the magnetic field $\kappa_{n,B}(x)$. It is natural to assume that

$$\kappa_{n,B} \neq 0 \ , \quad \text{on } \Gamma \ . \tag{1.6}$$

The case, where we can prove the full conjecture is the case when H is assumed to be orthogonal to Γ :

$$H \cdot T(x) = 0 \ , \ \forall x \in \Gamma \ , \tag{1.7}$$

where $T(x)$ is a unit tangent vector at x to Γ.
This occurs for example for an ellipsoid when H is parallel to one of the principal axis.

In this case, we shall show that :

$$\hat{\gamma}_0 = c_0 \inf_{x\in\Gamma} |\kappa_{n,B}(x)|^{\frac{2}{3}} \ , \tag{1.8}$$

where c_0 is a universal strictly positive constant attached to spectral invariants related to two model Hamiltonians respectively defined on $\mathbb{R}$ and $\mathbb{R}^+$ and which will be analyzed in Subsections 2.2 and 2.4.

Although the methods of proof can also lead to localization results for the ground state (see [HeMo2], [HeMo3]) or more generally for minimizers of the Ginzburg-Landau functional (see [HePa]), this will not be discussed here.

In Sections 2 and 3, we recall previous results extracted of [DaHe], [HeMo2], [LuPa5], [HeMo3], which will play an important role in the analysis. In Section 4, we recall the results of [LuPa5] devoted to the case when the magnetic field is not constant. It is also shown there that the problem is reduced in the constant magnetic case to a neighborhood of the boundary. In Section 5, we make explicit our choice of coordinates near the boundary. Section 6 gives rough upper bounds for the ground state energy by constructing quasimodes. In Section 7, we present our first lower bounds which are sufficiently accurate for giving the right order for the remainder. In Section 8, we go further in the choice of adapted coordinates, taking in particular account of the fact that the magnetic field is constant. This permits to introduce our magnetic invariants attached to Γ and to present in Section 9 our main results in a more precise form. Section 10 is devoted to the research of simpler models for the magnetic potentials obtained in the adapted coordinates by suitable gauge transformations and by neglecting "small" terms. Section 11 is devoted to the estimate of the errors done in the use of the previous models. In Section 12, we start by some heuristics which lead to the spectral analysis of a simplified model which will be used in the general case. Section 13 is devoted to the proof of the accurate upper bounds. We start with the analysis of the particular case, which is simpler, for helping the reader. Section 14 is devoted to the proof of accurate lower bounds, but in a particular case.

2 The case of dimension 2

2.1 Main results for the models with constant magnetic fields

We first consider the operator :

$$P_A^h := (hD_{x_1} - A_1)^2 + (hD_{x_2} - A_2)^2 \ ,$$

with $A = (-\frac{b}{2}x_2, \frac{b}{2}x_1)$, $h > 0$ and $b > 0$, and analyze the spectrum of its realization in $\mathbb{R}^2$ or of its Neumann realization in $\mathbb{R}^2_+$.

We observe that by homogeneity, one can reduce the analysis to $h = 1$ and $b = 1$. It is well known that in the case of $\mathbb{R}^2$ the spectrum is a point spectrum and that the eigenvalues are given by $(2n + 1)$ with $(n \in \mathbb{N})$, each eigenvalue being of infinite multiplicity. One way, to see this is to show the unitary equivalence (via a gauge transformation, a partial Fourier transform and a translation) with the harmonic oscillator $(-\partial_t^2 + t^2)$ but seen as an unbounded operator on $L^2(\mathbb{R}^2_{t,s})$.

The case of the Neumann realization in $\mathbb{R}^2_+$ is a little more delicate. A unitary transformation leads this time to the analysis of the Neumann realization of the operator of

$$Q(t, D_t; s) := D_t^2 + (t-s)^2 \text{ on } L^2(\mathbb{R}_+ \times \mathbb{R}) \tag{2.1}$$

which is reduced to the analysis of the family ($s \in \mathbb{R}$) of operators :

$$Q(s) := D_t^2 + (t-s)^2 \, , \tag{2.2}$$

defined on $L^2(\mathbb{R}_+)$.

If $\mu(s)$ is defined as the lowest eigenvalue of the Neumann realization of $Q(s)$ in $\mathbb{R}^+$, one easily shows (cf [ReSi])

Proposition 2.1 .
The infimum of the spectrum of the Neumann realization of P_A^h is given by $bh\Theta_0$ with :

$$\Theta_0 := \inf_{s \in \mathbb{R}} \mu(s) \, . \tag{2.3}$$

2.2 An important one-dimensional family of operators on $\mathbb{R}$

We recall the main properties of the groundstate energy of the Neumann realization on $\mathbb{R}^+$ of

$$Q(s) := D_t^2 + (t-s)^2 \, , \tag{2.4}$$

in function of the parameter $s \in \mathbb{R}$. Let us just list some properties of $\mu(s)$ and of the correspoing φ^s and refer to [DaHe], [HeMo2] for proofs or details. The Neumann eigenvalue $\mu(s)$ satisfies the following properties :

1. $\lim_{s \to -\infty} \mu(s) = +\infty$;
2. μ is decreasing for $s < 0$;
3. $\mu(0) = 1$;
4. $\lim_{s \to +\infty} \mu(s) = 1$;
5. μ admits in $]0, +\infty[$ a unique minimum $\Theta_0 < 1$ at some $\xi_0 > 0$. So

   $$\Theta_0 := \inf_{s \in \mathbb{R}} \mu(s) = \mu(\xi_0) < 1 \, . \tag{2.5}$$

   This minimum is non degenerate and more precisely :

   $$0 < \mu''(\xi_0) < 2 \, . \tag{2.6}$$

6. We introduce $\varphi_0 = \varphi^{\xi_0}$. We have :

   $$\int_{\mathbb{R}_+} (t - \xi_0) |\varphi_0(t)|^2 \, dt = 0 \, , \tag{2.7}$$

   which just corresponds to the condition $\mu'(\xi_0) = 0$.

7. φ_0 is rapidly decreasing at ∞.

Let us just mention that the proof of some of these properties is based on the following identity, relating the first eigenfunction φ^s and $\mu(s)$:

$$||\varphi^s||^2 \mu'(s) = (s^2 - \mu(s))(\varphi^s(0))^2 \, . \tag{2.8}$$

2.3 Applications: main results in dimension 2

As an application of the analysis of the models, one gets (cf [LuPa3]) via a partition of unity for the lower bound and a suitable construction of quasimodes for the upper bound, the following general result (in the two-dimensional case) :

Theorem 2.2 .
If $\lambda(h)$ is the lowest eigenvalue of the Neumann realization of P_A^h in Ω, then we have :

$$\lim_{h\to 0} \frac{\lambda(h)}{h} = \min \left(\inf_{x\in\Omega} |B(x)|, \Theta_0 \inf_{x\in\partial\Omega} |B(x)| \right) \, , \tag{2.9}$$

where $B = \mathrm{curl}\, A$.

We emphasize that there is no assumption that the magnetic field is constant. In the case of the constant magnetic field, one can actually have more precise results for $\lambda(h)$. When B is constant, the minimum in (2.9) is obtained by the second term and we show in [BeSt], [PiFeSt] and [HeMo2] the

Theorem 2.3 .
If the magnetic field is constant of intensity b, then :

$$\lambda(h) = b\Theta_0 h - c_1 b^{\frac{1}{2}} \left(\sup_{x\in\partial\Omega} \kappa(x) \right) h^{\frac{3}{2}} + o(h^{\frac{3}{2}}) \, , \tag{2.10}$$

where c_1 is a universal strictly positive universal constant and $\kappa(x)$ is the curvature of $\partial\Omega$ at $x \in \partial\Omega$.

2.4 The Montgomery's model and a second important family of operators on $I\!R$.

We just discuss a model that we shall meet indirectly later and which is interesting. It first appears in [Mon] but see also [HeMo1]. We consider in $I\!R^2_{x,y}$, and for some parameter $\gamma > 0$ the operator :

$$P := h^2 D_x^2 + (hD_y - \frac{\gamma}{2} x^2)^2 \, . \tag{2.11}$$

The magnetic potential is $\vec{A} = (0, \frac{\gamma}{2} x^2)$ and we have :

$$\mathrm{curl}\, A = \gamma x \, .$$

So the magnetic field vanishes along a line. Let us briefly describe the spectral analysis. After a Fourier transform in the y-variable, we first get :

$$\hat{P} = h^2 D_x^2 + (h\eta - \frac{\gamma}{2} x^2)^2 \ ,$$

and this leads to the analysis of the family, parametrized by $\eta \in I\!R$, of selfadjoint operators on $L^2(I\!R)$:

$$\hat{P}(\eta) = h^2 D_x^2 + (h\eta - \frac{\gamma}{2} x^2)^2 \ .$$

Using a simple dilation, we get :

$$\inf \text{ Sp } (\hat{P}) = \inf_{\eta} \inf \text{ Sp } (\hat{P}(\eta)) = h^{\frac{4}{3}} |\frac{\gamma}{2}|^{\frac{2}{3}} \inf_{\rho} \inf \text{Sp } (D_r^2 + (r^2 - \rho)^2) \ . \quad (2.12)$$

Let us recall some properties of the family of operators

$$S(\rho) = D_r^2 + (r^2 - \rho)^2 \ , \quad (2.13)$$

and of the corresponding ground state ψ^ρ, which were established in [Mon], [HeMo1] and [PaKw].

1. There exists a unique $\rho = \rho_{min}$ such that :

$$\hat{\nu}_0 := \inf_{\rho} \inf \text{ Sp } (D_r^2 + (r^2 - \rho)^2) = \inf \text{ Sp } (D_r^2 + (r^2 - \rho_{min})^2) \ . \quad (2.14)$$

2. ψ^ρ belongs to $\mathcal{S}(I\!R)$ and is even.

We shall later use the notation :

$$\psi_0 = \psi^{\rho_{min}} \ . \quad (2.15)$$

3 Constant magnetic field: models in $I\!R^3$ and in $I\!R^3_+$.

As in the case of dimension 2, where the first thing was to understand the model with constant magnetic feld in $I\!R^2$ and $I\!R^2_+$, we shall discuss the case of $I\!R^3$ and $I\!R^3_+$.

3.1 Model in $I\!R^3$.

We start (after some gauge transformation) of the Schrödinger operator with constant magnetic field in dimension 3.

$$P^h(\vec{H}) := h^2 D_{x_1}^2 + (hD_{x_2} - H_3 x_1)^2 + (hD_{x_3} + H_2 x_1 - H_1 x_2)^2 \ . \quad (3.1)$$

The following lemma has the age of quantum mechanics :

Lemma 3.1 .
The bottom of the spectrum of the selfadjoint realization of $P^h(\vec{H})$ in $\mathbb{R}^3$ is

$$\inf \mathrm{Sp} \left(P^{h,N}_{\mathbb{R}^3}(\vec{H}) \right) = bh \ , \tag{3.2}$$

where

$$b = || H || = \sqrt{H_1^2 + H_2^2 + H_3^2}$$

is the intensity of H.

3.2 Models in halfspaces.

We refer to [LuPa5] and [HeMo3] for the proof of the results presented in this subsection. If N is a unit vector in $\mathbb{R}^3$, we now consider the Neumann realization in $\Omega := \{x \in \mathbb{R}^3 \mid x \cdot N > 0\}$. After a rotation, we can assume in the proofs that $N = (1,0,0)$, so Ω is $\mathbb{R}^3_+ := \{x_1 > 0\}$.
After scaling, we can assume that $h = 1$ and $||H|| = 1$.

After some rotation in the (x_2, x_3) variables, we can assume that the new magnetic field is $(\beta_1, \beta_2, 0)$ and we are reduced to the problem of analyzing :

$$P(\beta_1, \beta_2) := D_{x_1}^2 + D_{x_2}^2 + (D_{x_3} + \beta_2 x_1 - \beta_1 x_2)^2 \ ,$$

in $\{x_1 > 0\}$, where :

$$\beta_1^2 + \beta_2^2 = 1 \ .$$

We introduce :

$$\beta_2 = \cos\vartheta \ , \ \beta_1 = \sin\vartheta \ ,$$

and we observe that, if N is the external normal to $x_1 = 0$, we have :

$$\vec{H} \cdot N = -\sin\vartheta \ . \tag{3.3}$$

By partial Fourier transform, we arrive to :

$$L(\vartheta, \tau) = D_{x_1}^2 + D_{x_2}^2 + (\tau + \cos\vartheta \ x_1 - \sin\vartheta \ x_2)^2 \ , \tag{3.4}$$

in $x_1 > 0$ and with Neumann condition on $x_1 = 0$. The bottom of the spectrum of $L(\vartheta, \tau)$ is given by :

$$\sigma(\vartheta) := \inf \ \mathrm{Sp} \ (L(\vartheta, D_t)) = \inf_{\tau} (\inf \ \mathrm{Sp} \ (L(\vartheta, \tau))) \ . \tag{3.5}$$

Proposition 3.2 .
The bottom of the spectrum of the Neumann realization of $P^h(\vec{H})$ in $\Omega := \{x \in \mathbb{R}^3 \mid x \cdot N > 0\}$ is :

$$\inf \ \mathrm{Sp} \, P^{h,N}_{\Omega}(\vec{H}) = \sigma(\vartheta) \ b \ h \ , \tag{3.6}$$

where $\vartheta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ is defined by (3.3).

By symmetry considerations, we observe also that :

$$\sigma(\vartheta) = \sigma(-\vartheta) = \sigma(\pi - \vartheta) \ . \tag{3.7}$$

It is consequently enough to look at the restriction to $[0, \frac{\pi}{2}]$.

3.3 Properties of $\vartheta \mapsto \sigma(\vartheta)$.

Let us now list the main properties of the function $\vartheta \mapsto \sigma(\vartheta)$ on $[0, \frac{\pi}{2}]$. Most of them are established in [LuPa5] but see also [HeMo3].

1. σ is continuous on $[0, \frac{\pi}{2}]$.
2. $$\sigma(0) = \Theta_0 < 1 \ . \tag{3.8}$$
3. $$\sigma(\frac{\pi}{2}) = 1 \ . \tag{3.9}$$
4. $$\sigma(\vartheta) \geq \Theta_0 (\cos\vartheta)^2 + (\sin\vartheta)^2 \ . \tag{3.10}$$
5. If $\vartheta \in]0, \frac{\pi}{2}[$, the spectrum of $L(\vartheta, \tau)$ is independent of τ and its essential spectrum is contained in $[1, +\infty[$.
6. For $\vartheta \in]0, \frac{\pi}{2}[$, $\sigma(\vartheta)$ is an isolated eigenvalue of $L(\vartheta, \tau)$, with finite multiplicity.
7. The function σ is strictly increasing on $[0, \frac{\pi}{2}[$.
8. The function σ has the following expansion for ϑ small :
$$\sigma(\vartheta) \sim \Theta_0 + \sum_{n \geq 1} \alpha_n |\vartheta|^n \ , \tag{3.11}$$
with $\alpha_1 = \sqrt{\frac{\mu''(\xi_0)}{2}} > 0$.

A first consequence of this analysis is

Proposition 3.3 .
When $b = ||H||$ is fixed the bottom of the spectrum of $P_\Omega^{h,N}(\vec{H})$ in $\Omega := \{x \cdot N > 0\}$ is minimal when $\vartheta = 0$ that is, according to (3.3), that is when the magnetic field vector satisfies $\vec{H} \cdot N = 0$.

4 First results for general magnetic fields

In the case of dimension 2, under the assumption that $\operatorname{curl} A := B(x) > 0$, the basic estimate at the interior was the inequality :

$$h \int B(x) |u(x)|^2 dx \leq \int |(h\nabla - iA)u|^2 dx \ , \ \forall u \in C_0^\infty(\Omega) \ . \tag{4.1}$$

This was not enough for understanding the Neumann problem. One should more carefully analyze the case of $\mathbb{R}^2_+$ and, in the case of the constant magnetic field, one should also analyze more complicate models (like for example the case of the disk). The most spectacular result was :

Theorem 4.1 .
When the magnetic field is constant, the groundstate of the Neumann realization of P_A^h in an open regular bounded set $\Omega \subset I\!R^2$ is localized in the neighborhood of the points of the boundary of maximal curvature.

In the case of dimension 3, estimate (4.1) should be replaced by the weaker estimate established in [HeMo1] (Theorem 3.1)

Theorem 4.2 .
There exist C and $h_0 > 0$ such that, for all $h \in]0, h_0]$, we have :

$$h \int_\Omega (||H(x)|| - Ch^{\frac{1}{4}})|u(x)|^2 dx \leq \int_\Omega |(h\nabla - iA)u|^2 dx \ , \ \forall u \in C_0^\infty(\Omega) \qquad (4.2)$$

If this result is essentially sufficient for analyzing the Dirichlet problem in Ω, it is necessary to implement the analysis given in the first part in order to treat the Neumann problem. Near each point of the boundary x, we have to use the lower bound obtained for the model with constant magnetic field $H = H(x)$. Following for example the proof in [HeMo2] and using the same partition of unity, we get :

Theorem 4.3 .

$$h \int_\Omega W_h(x)|u(x)|^2 dx \leq \int |(h\nabla - iA)u|^2 dx \ , \ \forall u \in H^1(\Omega) \qquad (4.3)$$

where

$$\begin{array}{lll} W_h(x) & = ||H(x)|| - Ch^{\frac{1}{4}} \ , & \text{if } d(x, \partial\Omega) \geq 2h^{\frac{3}{8}} \ , \\ & = ||H(s(x))||\ \sigma(\vartheta(x) - Ch^{\frac{1}{4}} & \text{if } d(x, \partial\Omega) \leq 2h^{\frac{3}{8}} \ . \end{array} \qquad (4.4)$$

Here we recall that $\vartheta(x)$ satisfies :

$$||H(s(x))|| \cdot \sin\vartheta(x) = -H(s(x)) \cdot N(s(x)) \ , \qquad (4.5)$$

where $s(x)$ is, for x near $\partial\Omega$, the point in $\partial\Omega$ such that :

$$d(x, \partial\Omega) = d(x, s(x)) \ ,$$

and we observe that, due to (3.7), $\sigma(\vartheta(x))$ is well defined by (4.5).
The first consequence (compare with Theorem 2.2) is :

Theorem 4.4 .

$$\lim_{h\to 0} (\lambda(h)/h) = \min \left(\inf_{x\in\Omega} ||H(x)|| \ , \ \inf_{x\in\partial\Omega} ||H(x)||\ \sigma(\vartheta(x)) \right) \ . \qquad (4.6)$$

The lower bound is a direct consequence of Theorem 4.3 and the proof of the upper bound is sketched in [LuPa5]. When $H(x)$ is constant of intensity b , then the minimum in (4.6) is obtained for the second term and we have :

$$\lim_{h\to 0} (\lambda(h)/h) = b \left(\inf_{x\in\partial\Omega} \sigma(\vartheta(x)) \right) \ . \qquad (4.7)$$

But it should be (see (6.3)) one point such that $\vartheta(x) = 0$, so we get :

$$\lim_{h\to 0} (\lambda(h)/h) = \Theta_0 b\,. \tag{4.8}$$

Remark 4.5 .
As in [HeMo2], this leads to localization theorems ([LuPa5], [HeMo3] but see also [PiFeSt]). In particular, if the magnetic field is constant, then the ground state is localized near the points of the boundary where the magnetic field is parallel to the tangent space.

Application.
An interesting case is the case when H is constant and when Ω is the ellipsoid :

$$a_1 x_1^2 + a_2 x_2^2 + a_3 x_3^2 \leq 1\,.$$

The set of points where $\vec{H} = (H_1, H_2, H_3)$ is parallel is obtained by intersecting the boundary of the ellipsoid with the plane :

$$a_1 x_1\, H_1 + a_2 x_2 H_2 + a_3 x_3 H_3 = 0\,.$$

More generally, if the surface is strictly convex and if the magnetic field is constant, it is possible to show that the set of points of the boundary where H is parallel to the tangent space is a C^∞ curve.

We emphasize that Theorem 4.4 does not explain all the situation. In the case with constant magnetic field it would be nice to show the role of some curvature in the localization as in the case of dimension 2. **This is actually our goal to give an answer to this question.**

5 Adapted coordinates

5.1 Magnetic geometrical invariants

The standard coordinates on $I\!R^3$ will be denoted by $x = (x_1, x_2, x_3)$ and the standard flat metric by g_0. We will also use $< \ . \mid . \ >$ for $g_0(\ .\ ,\ .\ )$ or for $g_0^\star(\ .\ ,\ .\ )$, and $|X|$ for $(< X|X >)^{\frac{1}{2}}$, (if X is a vector field or a one-form). The standard volume on $I\!R^3$ will be denoted by $\omega_3 = dx^3 = dx_1 \wedge dx_2 \wedge dx_3$ and will fix also the orientation of $I\!R^3$.

Let A be a smooth magnetic potential one-form on $\overline{\Omega}$, :

$$A = \sum_{j=1}^{3} A_j(x) dx_j, \quad A_j \ \in \ C^\infty(\overline{\Omega}; I\!R).$$

The magnetic field B is the two-form:

$$B = dA = \sum_{1\leq i<j\leq 3} B_{ij}(x) dx_i \wedge dx_j, \quad B_{ij}(x) = \frac{\partial A_j}{\partial x_i}(x) - \frac{\partial A_i}{\partial x_j}(x)\,. \tag{5.1}$$

If needed B_{ij} is extended as an antisymmetric matrix. The intensity of the magnetic field is the non negative function

$$|B|(x) = \sup\{|B_x(X,Y)|;\ X,\ Y\ \in\ T_x\overline{\Omega},\ |X| = |Y| = 1\},\quad \forall\, x\ \in\ \overline{\Omega}. \tag{5.2}$$

One associates to the magnetic field B, a vector field $\vec{H} := V(B)\ \in\ T\overline{\Omega}$ by

$$B_x(X,Y) = \omega_3(X,Y,V_x(B)),\quad \forall\ X,\ Y\ \in\ T_x\overline{\Omega}\,. \tag{5.3}$$

In the initial coordinates, we have :

$$V(B) = \sum_{j=1}^{3} b_j(x)\frac{\partial}{\partial x_j},\quad \text{with}\ \ b_1 = B_{23},\ b_2 = B_{31}\ \text{and}\ b_3 = B_{12}\,. \tag{5.4}$$

Then the magnetic intensity satisfies :

$$|B| = |V(B)|\,. \tag{5.5}$$

We associate to the magnetic potential A the sesquilinear form on $H^1(\Omega)$:

$$u \mapsto q_A^h(u) = \int_\Omega |\sqrt{-1}hdu + uA|^2\, dx^3\,. \tag{5.6}$$

Here $h\ \in\ ]0,+\infty[$ is a parameter. The associated differential operator is the magnetic Laplacian which is given in the standard coordinates by

$$P_A^h = (hD - A)^2 = \sum_{j=1}^{3}(hD_{x_j} - A_j(x))^2\,. \tag{5.7}$$

5.2 Local coordinates

If $y = (y_1, y_2, y_3)$ are new local coordinates, that is, if $\mathcal{V}_{x_0}$ is a neighborhood of some point $x_0\ \in\ \Omega$ and if $x \mapsto y = \Phi(x)$ is a diffeomorphism of $\mathcal{V}_{x_0}$ onto $\mathcal{O} \subset I\!R^3$, then in the new basis $(\frac{\partial}{\partial y_1}, \frac{\partial}{\partial y_2}, \frac{\partial}{\partial y_3})$ of $T\mathcal{V}_{x_0}$, the standard metric g_0 and the volume ω_3 becomes

$$g_0 = \sum_{1\le i,j\le 3} g_{ij}dy_i \otimes dy_j\,, \tag{5.8}$$

and

$$\omega_3 = |g|^{\frac{1}{2}}dy_1 \wedge dy_2 \wedge dy_3, \tag{5.9}$$

with

$$\begin{array}{ll} g_{ij} & =< \frac{\partial x}{\partial y_i}|\frac{\partial x}{\partial y_j} >\,, \\ < X|Y > & = \sum_{1\le i,j\le 3} g_{ij}\widetilde{X}_i\widetilde{Y}_j\,, \\ |g| & = \det(g_{ij})\,, \end{array}$$

where $X = \sum_j \widetilde{X}_j \frac{\partial}{\partial y_j}$ and $Y = \sum_j \widetilde{Y}_j \frac{\partial}{\partial y_j}$.
The magnetic potential is given in the new coordinates by

$$A = \sum_{j=1}^{3} \widetilde{A}_j dy_j \quad \text{with} \quad \widetilde{A}_j = \sum_{k=1}^{3} A_k \frac{\partial x_k}{\partial y_j}. \tag{5.10}$$

The magnetic field is also given by

$$B = \sum_{1 \le i < j \le 3} \widetilde{B}_{ij} dy_i \wedge dy_j \quad \text{with} \quad \widetilde{B}_{ij} = \frac{\partial \widetilde{A}_j}{\partial y_i} - \frac{\partial \widetilde{A}_i}{\partial y_j}. \tag{5.11}$$

So the vector magnetic field becomes

$$V(B) = \sum_{j=1}^{3} \widetilde{b}_j \frac{\partial}{\partial y_j} \ , \tag{5.12}$$

with

$$\widetilde{b}_1 = |g|^{-\frac{1}{2}} \widetilde{B}_{23} \ , \ \widetilde{b}_2 = |g|^{-\frac{1}{2}} \widetilde{B}_{31} \ , \ \widetilde{b}_3 = |g|^{-\frac{1}{2}} \widetilde{B}_{12} \ , \tag{5.13}$$

and the intensity of the magnetic field becomes :

$$|B| = (\sum_{i,j} g_{ij} \widetilde{b}_i \widetilde{b}_j)^{\frac{1}{2}} \ . \tag{5.14}$$

The sesquilinear form takes the following form, for u supported in $\mathcal{V}_{x_0}$,

$$q_A^h(u) = \int_{\mathcal{V}_{x_0}} |g|^{\frac{1}{2}} \sum_{1 \le i,j \le 3} g^{ij} [hD_{y_i} u - \widetilde{A}_i u] \times \overline{[hD_{y_j} u - \widetilde{A}_j u]} \, dy^3 \ , \tag{5.15}$$

and the associated differential operator is

$$P_A^h = |g|^{-\frac{1}{2}} \sum_{1 \le i,j \le 3} (hD_{y_j} - \widetilde{A}_j) \cdot |g|^{\frac{1}{2}} g^{ij} (hD_{y_i} - \widetilde{A}_i) \ . \tag{5.16}$$

Here g^{ij} is the inverse matrix of the matrix g_{ij}.

5.3 Adapted local coordinates near the boundary

Let $\phi(x) = (y_1, y_2)$ be local coordinates on the boundary and G the induced metric by g_0 on $\partial\Omega$ in these coordinates.. Then for $\epsilon > 0$ small enough (and modifying a little $\mathcal{V}_{x_0}$ if necessary), we can define local coordinates on $\mathcal{V}_{x_0}$,

$$\Phi \ : \ \mathcal{V}_{x_0} \ \to \ \mathcal{S} \times]0, \epsilon[, \quad \Phi(x) = (y_1, y_2, y_3)$$

such that

$$y_3(x) = \ \text{dist} \ (x, \phi^{-1}(y_1, y_2)) = \ \text{dist} \ (x, \partial\Omega); \tag{5.17}$$

so

$$x = \phi^{-1}(y_1, y_2) + y_3 N(\phi^{-1}(y_1, y_2)), \quad \forall\ x\ \in\ \mathcal{V}_{x_0}, \tag{5.18}$$

where $N(x)$ is the interior normal unit to $\partial\Omega$ at the point $x\ \in\ \partial\Omega$.
Then we get by simple computation the form of the standard flat metric g_0 in these new coordinates,

$$\begin{array}{rl} g_0 & = \sum_{1\leq i,j\leq 3} g_{ij}\, dy_i \otimes dy_j \\ & = dy_3 \otimes dy_3 + G \\ & \quad +2y_3 \sum_{1\leq i,j\leq 2} < \frac{\partial N}{\partial y_i} | \frac{\partial x}{\partial y_j} > dy_i \otimes dy_j \\ & \quad +y_3^2 \sum_{1\leq i,j\leq 2} < \frac{\partial N}{\partial y_i} | \frac{\partial N}{\partial y_j} > dy_i \otimes dy_j\ . \end{array} \tag{5.19}$$

In this case we have, using (5.10) and (5.18),

$$\widetilde{A}_3 = \sum_{j=1}^{3} A_j N_j\ .$$

Remark 5.1 .
In the following, we choose a finite family of open sets $\mathcal{V}_{x_j}$ ($x_j \in \partial\Omega$) covering a tubular neighborhood of $\partial\Omega$. When we shall speak later of local coordinates, we will mean that we take some element belonging to the family.

6 Rough upper bounds

To prove our results, we need some rough preliminary estimates (with some control of the remainder) of the ground state energy.

Proposition 6.1 .
Let Ω be a bounded open set of $\mathbb{R}^3$ with smooth boundary $\partial\Omega$. Let $P_{A,\Omega}^{h,N}$ be the Neumann operator on $L^2(\Omega)$ associated to the Schrödinger operator with constant magnetic field $(hD - A)^2$ and let us assume that the vector magnetic field $H = \mathrm{curl}\,(A)$ is constant.
If $\lambda(h) = \inf \mathrm{Sp}\,(P_{A,\Omega}^{h,N})$ is the first eigenvalue of $P_{A,\Omega}^{h,N}$, then there exists a constant C_0 such that

$$\lambda(h) \leq b\Theta_0 h + C_0 h^{\frac{4}{3}}\ . \tag{6.1}$$

Remark 6.2 .
It is not necessary to assume that the magnetic field is constant as the proof of this proposition will show. If one choose a point x_0 such that $H(x_0)$ is tangent to $\partial\Omega$, one can get the same result with $b = ||\, H(x_0)\,||$. One can then optimize by choosing a point of this kind such that $|B(x_0)|$ is minimal. If Γ is the set introduced in (1.4) we will prove :

$$\lambda(h) \leq \Theta_0 \inf_{x\in\Gamma} |H(x)|\, h + C_0 h^{\frac{4}{3}}\ . \tag{6.2}$$

Proof of Proposition 6.1.
As the flux of the magnetic field through the boundary is zero,

$$\int_{\partial\Omega} \mathrm{curl}\,(A(x)) \cdot N(x) ds = \int_{\Omega} \mathrm{div}\,\mathrm{curl}\,(A) dx = 0\ , \tag{6.3}$$

if N is the interior normal unit of $\partial\Omega$, there exists $x_0 \in \partial\Omega$ such that the vector magnetic field is tangent to $\partial\Omega$ at x_0:

$$\mathrm{curl}\,(A(x_0)) \cdot N(x_0) = 0.$$

We take local coordinates (y_1, y_2) in a neighbourhood of W_0 of x_0 in $\partial\Omega$ such that the metric is δ_{ij} at x_0 and $\frac{\partial}{\partial y_1}$ is parallel to the vector magnetic field.
We consider the adapted coordinates $y = (y_1, y_2, y_3)$, with $y_3(x) = d(x, \partial\Omega)$, and then $g_{ij}(x_0) = \delta_{ij}$. If $\widetilde{A}$ is the magnetic potential in the new coordinates, $A \cdot dx = \widetilde{A} \cdot dy$, then

$$\begin{array}{l} \frac{\partial \widetilde{A}_3}{\partial y_2}(x_0) - \frac{\partial \widetilde{A}_2}{\partial y_3}(x_0) = b \\ \frac{\partial A_1}{\partial y_3}(x_0) - \frac{\partial A_3}{\partial y_1}(x_0) = 0 \\ \frac{\partial A_2}{\partial y_1}(x_0) - \frac{\partial A_1}{\partial y_2}(x_0)) = 0\ . \end{array} \tag{6.4}$$

We can find a a gauge transform $\exp i\frac{\varphi}{h}$, with φ real, such that, in (8.27),

$$\widetilde{A}_1(x_0) = 0\ ,\ \widetilde{A}_2(x_0) = 0\ ,\ \widetilde{A}_3 = 0\ .$$

We first estimate the error occuring when eliminating the terms vanishing to order 3.
If $u \in H^1(\Omega)$ is such that

$$\mathrm{supp}(u) \subset \{x;\ |x - x_0| \leq h^\delta\} \tag{6.5}$$

with $\delta > 0$, and if h is small enough, then, for some $C > 0$,

$$q_A^h(e^{i\frac{\varphi}{h}}u) \leq (1 + h^\delta C) q_{A^0}^h(u) + C[h^{3\delta}(q_{A^0}^h(u))^{\frac{1}{2}} \cdot \|u\| + h^{6\delta}\|u\|^2]\ , \tag{6.6}$$

where

$$A_1^0 = R_1(y),\ A_2^0 = -by_3 + R_2(y),\ A_3^0 = 0\ ,$$

the $R_j(y)$ are polynomial functions, homogeneous of order two,

$$R_j(y) = \sum_{|\alpha|=2} a_{j,\alpha} y^\alpha,$$

and

$$q_{A^0}^h(u) = \int_{|y| \leq Ch^\delta,\ y_3 > 0} |(hD_y u - A^0(y)u|^2\ dy\ . \tag{6.7}$$

We take the function u in the form

$$u(y_1, y_2, y_3) := e^{-ib^{\frac{1}{2}} y_2 \xi_0 / h^{\frac{1}{2}}} v(y)$$

with

$$v(y_1,y_2,y_3) = h^{-\frac{1}{4}-\delta}\varphi_0(b^{\frac{1}{2}}h^{-\frac{1}{2}}y_3)\chi(4h^{-\delta}y_3)\chi(4h^{-\delta}(y_1^2+y_2^2)^{\frac{1}{2}}) \ . \tag{6.8}$$

Here χ is a cut off function equal to one on $[-\frac{1}{2},\frac{1}{2}]$ and supported in $[-1,1]$, φ_0 is introduced in Subsection 2.2 and $\delta \in]0,\frac{1}{2}[$.
Observing that :

$$\int_{I\!R_+} (|D_t\varphi_0(t)|^2 + |(t-\xi_0)\varphi_0(t)|^2)dt = \Theta_0 \int_{I\!R_+} |\varphi_0(t)|^2 dt,$$

and that $t \mapsto \varphi_0(t)$ is an exponentially decreasing function at infinity,
we get when $\delta = \frac{1}{3}$,

$$q^h_{\hat{A}^0}(u) \leq (b\Theta_0 h + C\, h^{\frac{4}{3}})\|u\|^2 \ , \tag{6.9}$$

where

$$\hat{A}^0_1 = 0,\ \hat{A}^0_2 = -by_3,\ \hat{A}^0_3 = 0 \ .$$

We then have to compare $q^h_{\hat{A}^0}(u)$ and $q^h_{A^0}(u)$. The first try could be to use :

$$q^h_{A^0}(e^{i\frac{\varphi}{h}}u) \leq (1+h^\delta C)q^h_{\hat{A}^0}(u) + C[h^{2\delta}(q^h_{\hat{A}^0}(u))^{\frac{1}{2}}\cdot\|u\| + h^{4\delta}\|u\|^2] \ , \tag{6.10}$$

This leads to error terms of size $h^{1+\delta}$, $h^{\frac{1}{2}+2\delta}$, $h^{4\delta}$ and $h^{2-2\delta}$. But this leads only, using (6.9) and (6.10) with $\delta = \frac{1}{3}$, to (6.1) with $\mathcal{O}(h^{\frac{7}{6}})$ instead of $\mathcal{O}(h^{\frac{4}{3}})$ as expected.

In order to get effectively (6.1), we need to use (2.7). We have indeed to analyze more carefully the term which was bounded from above in (6.10) by $h^{2\delta}(q^h_{\hat{A}^0}(u))^{\frac{1}{2}}\cdot\|u\|$.

The terms which were estimated by $h^{\frac{1}{2}+2\delta}$ are of the form

$$h^{-\frac{1}{2}-2\delta}\int y_jy_k(\xi_0 - \frac{b^{\frac{1}{2}}y_3}{h^{\frac{1}{2}}})\varphi_0^2(b^{\frac{1}{2}}h^{-\frac{1}{2}}y_3)\chi^2(4h^{-\delta}(y_1^2+y_2^2)^{\frac{1}{2}})dy \ ,$$

with j and k equal to 1 or 2. But they actually vanish due to (2.7).

The other terms have actually better upper bounds. We observe indeed that for example :

$$h^{-\frac{1}{2}-2\delta}\int y_2y_3(\xi_0 - \frac{b^{\frac{1}{2}}y_3}{h^{\frac{1}{2}}})\varphi_0^2(b^{\frac{1}{2}}h^{-\frac{1}{2}}y_3)\chi(h^{-\delta}y_3)\chi^2(4h^{-\delta}(y_1^2+y_2^2)^{\frac{1}{2}})dy \ ,$$

can be estimated by $\mathcal{O}(h^{1+\delta})$.

This suggests strongly that the next term in the expansion of $\lambda(h)$ is $\mathcal{O}(h^{\frac{4}{3}})$, but to go further we need to analyze the model more carefully in the neighborhood of the points of the boundary where $H(x)\cdot N(x)$ vanishes. For this we need to enter more deeply in the geometry of the boundary in connection with the magnetic vector field, and this will be done in Section 8.

7 Rough lower bounds

We assume that the magnetic field is constant. Let u^h be an eigenfunction associated to the eigenvalue $\lambda(h) = \inf\ \mathrm{Sp}\ (P^{h,N}_{A,\Omega})$.

7.1 A priori estimates

As proved in [HeMo2], we have, without the assumption (1.5), the following behavior of u^h.

Proposition 7.1 .
If $t = t(x) = d(x, \partial\Omega)$, then, for any $k \in I\!N$, there exists a constant C_k depending only on k, such that

$$\|t^{\frac{k}{2}} u^h\| \leq C_k h^{\frac{k}{4}} \|u^h\| \tag{7.1}$$

and

$$\|t^{\frac{k}{2}} (hD - A)u^h\| \leq C_k h^{(k+2)/4} \|u^h\| \,. \tag{7.2}$$

Proof of Proposition 7.1 .
Proposition 6.1 and the fact that $\Theta_0 < 1$, give the existence of $h_0 > 0$ and of a constant $C_0 > 1$ such that

$$C_0^{-1} bh \leq bh - \lambda(h) \leq C_0 bh \,. \tag{7.3}$$

Of course this a very rough estimate.

Let us remark that (7.1) and (7.2) are valid when $k = 0$. As for the 2-dimensional case in [HeMo1], we proceed by recursion.
By changing t away from the boundary, we can assume that $x \mapsto t(x) = d(x, \partial\Omega)$ is extended as a $C^1(\overline{\Omega})$ function. By choosing suitable coordinates and after a gauge transform, we can assume that

$$A_1(x) = 0, \quad A_2(x) = -\frac{b}{2} x_3, \quad A_3(x) = \frac{b}{2} x_2 \,.$$

As $t/\partial\Omega = 0$, we have by integrating by parts and for $k > 0$,

$$\begin{array}{l} ihb \int_\Omega t^k |u^h|^2 dx = \int_\Omega t^k [(hD_2 - A_2), (hD_3 - A_3)] u^h \ \cdot\ \overline{u}^h dx \\ = \int_\Omega t^k \{(hD_3 - A_3)u^h \overline{(hD_2 - A_2)u^h} - (hD_2 - A_2)u^h \overline{(hD_3 - A_3)u^h}\} dx \\ + ihk \int_\Omega t^{k-1} \{\frac{\partial t}{\partial x_2}(hD_3 - A_3)u^h - \frac{\partial t}{\partial x_3}(hD_2 - A_2)u^h\} \overline{u}^h dx \end{array} \tag{7.4}$$

and

$$\int_\Omega t^k |(hD - A)u^h|^2 dx = \int_\Omega \{\lambda(h) t^k |u^h|^2 - ihk t^{k-1} ((\nabla_x t) \cdot (hD - A)u^h) \overline{u}^h\} dx \,. \tag{7.5}$$

If $k = 1$ we get from (7.4)

$$hb \int_\Omega t |u^h|^2 dx \leq \int_\Omega t |(hD - A)u^h|^2 dx + Ch \|(hD - A)u^h\| \cdot \|u^h\| \,, \tag{7.6}$$

and then, we use (7.5) to get

$$hb\int_\Omega t|u^h|^2dx \le \lambda(h)\int_\Omega t|u^h|^2dx + Ch\|(hD-A)u^h\|\cdot\|u^h\| \ . \tag{7.7}$$

So

$$(hb-\lambda(h))\int_\Omega t|u^h|^2dx \le Ch\sqrt{\lambda(h)}\|u^h\|^2 \ . \tag{7.8}$$

We obtain (7.1) with $k=1$ from (7.3) and (7.8), and then it is easy to get (7.2) for $k=1$ from (7.5) using (7.3), (7.1) with $k=1$ and (7.2) with $k=0$.
If $k \ge 2$, we get in the same way

$$(hb-\lambda(h))\int_\Omega t^k|u^h|^2dx \le hkC\|t^{-1+\frac{k}{2}}(hD-A)u^h\|\cdot\|t^{\frac{k}{2}}u^h\| \ , \tag{7.9}$$

which gives, using (7.3),

$$\|t^{\frac{k}{2}}u^h\| \le Ck\|t^{-1+\frac{k}{2}}(hD-A)u^h\| \ . \tag{7.10}$$

Using (7.10) and (7.5) we get

$$\|t^k|(hD-A)u^h\|^2 \le Ckh[\|t^{\frac{k}{2}}u^h\|^2 + \|t^{-1+\frac{k}{2}}|(hD-A)u^h\|^2] \ . \tag{7.11}$$

Then we can proceed by recursion. (7.2) for $k=j-2$ and (7.10) for $k=j$ give (7.1) for $k=j$. Formulas (7.11) with $k=j$ and (7.2) for $k=j-2$ give (7.2) with $k=j$.

7.2 A partition of unity

Let $(\chi_\gamma(z))_{\gamma\in\mathbb{Z}^3}$ be a partition of unity of $\mathbb{R}^3$. For example we can take

$$\chi_\gamma \in C^\infty(\mathbb{R}^3;\mathbb{R}) \text{ and } \mathrm{supp}(\chi_\gamma) \subset \gamma+[-1,1]^3,\ \forall\gamma\in\mathbb{Z}^3,$$

$$\sum_\gamma \chi_\gamma^2(z) = 1 \text{ and } \sum_\gamma |\bigtriangledown\chi_\gamma(z)|^2 \ < \ \infty. \tag{7.12}$$

If $\tau(h)$ is a function of h such that $\tau(h)\in]0,\epsilon(\Omega)[$, where $\epsilon(\Omega)$ is the geometric constant which is the maximal ϵ for the property that $\{d(x,\partial\Omega)<\epsilon\}$ is a regular tubular neighborhood in $\overline{\Omega}$ of $\partial\Omega$, we will define the functions

$$\chi_{\gamma,\tau(h)}(z) = \chi_\gamma(z/\tau(h)), \quad \forall\,\gamma\ \in\ \mathbb{Z}^3 \ . \tag{7.13}$$

So we get a new partition of unity such that

$$\sum_\gamma \chi^2_{\gamma,\tau(h)}(z) = 1, \quad \sum_\gamma |\nabla\chi_{\gamma,\tau(h)}(z)|^2 \le C\,\tau(h)^{-2} \ , \tag{7.14}$$

and

$$\mathrm{supp}(\chi_{\gamma,\tau(h)}) \subset \tau(h)\gamma+[-\tau(h),\tau(h)]^3.$$

Then, for any $u \in H^1(\Omega)$, we have :

$$q_A^h(u) = \sum_\gamma \left[q_A^h(\chi_{\gamma,\tau(h)} u) - h^2 \| \, |\nabla \chi_{\gamma,\tau(h)}| \, u \, \|^2 \right] \ . \tag{7.15}$$

Let us define

$$\begin{array}{l} \Gamma_{\tau(h)}(\Omega) = \{\gamma \in \mathbb{Z}^3; \ \mathrm{supp}(\chi_{\gamma,\tau(h)}) \cap \Omega \neq \emptyset\} \\ \Gamma^0_{\tau(h)}(\Omega) = \{\gamma \in \Gamma_{\tau(h)}(\Omega); \ \ \mathrm{dist}\ (\mathrm{supp}(\chi_{\gamma,\tau(h)}), \partial\Omega) > \tau(h)\} \\ \Gamma^1_{\tau(h)}(\Omega) = \{\gamma \in \Gamma_{\tau(h)}(\Omega); \ \ \mathrm{dist}\ (\mathrm{supp}(\chi_{\gamma,\tau(h)}), \partial\Omega) \leq \tau(h)\} \end{array} \tag{7.16}$$

7.3 Proof of Theorem 1.1: Lower bounds

For the moment, we give a rough lower bound of the ground state energy in the case of constant magnetic field.

Proposition 7.2 .
Under the assumptions of Proposition 6.1, there exists C_0 such that :

$$b\Theta_0 h - C_0 h^{\frac{4}{3}} \leq \lambda(h) \ . \tag{7.17}$$

Proof of Proposition 7.2 .
We proceed as in the proof of Proposition 9.2 of [HeMo2] and use the partition of unity introduced in the previous subsection.

Far from the boundary .
As curl A is constant, the standard estimate gives :

$$\|(hD - A)w\|^2_{L^2(\mathbb{R}^3)} \geq bh \|w\|^2_{L^2(\mathbb{R}^3)} \ , \ \forall \ w \in C_0^\infty(\mathbb{R}^3) \ .$$

So

$$q_A^h(\chi_{\gamma,\tau(h)} u) \geq bh \|\chi_{\gamma,\tau(h)} u\|^2 \ , \ \forall \ \gamma \in \Gamma^0_{\tau(h)}(\Omega) \ . \tag{7.18}$$

Near the boundary .
Suppose $\gamma \in \Gamma^1_{\tau(h)}(\Omega)$; then there exists local coordinates[3] adapted to the boundary $y = (y_1, y_2, y_3)$ such that $y_3(x) = d(x, \partial\Omega)$.

Then, for $\tau(h) < 1$ and for some integer $k \in \mathbb{N}^\star$,

$$\begin{array}{rl} q_A^h(\chi_{\gamma,\tau(h)} u) & \geq (1 - C\tau(h)) q^h_{\widetilde{A}^{(k)}}(\chi_{\gamma,\tau(h)} u) \\ & \quad - C(\tau(h))^{k+1} \|\chi_{\gamma,\tau(h)} u\| \cdot (q_A^h(\chi_{\gamma,\tau(h)} u))^{1/2} \\ & \quad - C(\tau(h))^{2k+2} \|\chi_{\gamma,\tau(h)} u\|^2 \ , \end{array} \tag{7.19}$$

with, for some $y_0 \in \partial\Omega \cap \{\tau(h) + \mathrm{supp}(\chi_{\gamma,\tau(h)})\}$,

$$\widetilde{A}^{(k)} = \widetilde{A}(y_0) + \sum_{1 \leq |\alpha| \leq k} (y - y_0)^\alpha \frac{\partial^\alpha \widetilde{A}}{\partial y^\alpha}(y_0)$$

[3] belonging to the family introduced in Subsection 5.3

and

$$
\begin{aligned}
&q^h_{\widetilde{A}^{(k)}}(w)\\
&= |g|^{1/2}(y_0)\int_{I\!R^2\times I\!R_+}[\,|(hD_{y_3}-\widetilde{A}_3^{(k)})w|^2\\
&\quad+\textstyle\sum_{1\le i,j\le 2} g^{ij}(y_0)(hD_{y_i}-\widetilde{A}_i^{(k)})w\cdot\overline{(hD_{y_j}-\widetilde{A}_j^{(k)})w}]dy\ .
\end{aligned}
$$

Let us remark that

$$
\|\chi_{\gamma,\tau(h)}u\|^2 \le (1+C\tau(h))|g|^{1/2}(y_0)\int_{I\!R^2\times I\!R_+}|\chi_{\gamma,\tau(h)}u|^2dy\ , \tag{7.20}
$$

and by (5.12)

$$
b^2 = |g|^{-1}(y_0)[(\widetilde{H}_3^0)^2+\sum_{1\le j,k\le 2} g^{jk}(y_0)\widetilde{H}_j^0\widetilde{H}_k^0] \tag{7.21}
$$

if

$$
\begin{aligned}
\widetilde{H}_1^0 &= \tfrac{\partial\widetilde{A}_3}{\partial y_2}(y_0)-\tfrac{\partial\widetilde{A}_2}{\partial y_3}(y_0),\\
\widetilde{H}_2^0 &= \tfrac{\partial\widetilde{A}_1}{\partial y_3}(y_0)-\tfrac{\partial\widetilde{A}_3}{\partial y_1}(y_0),\\
\widetilde{H}_3^0 &= \tfrac{\partial\widetilde{A}_2}{\partial y_1}(y_0)-\tfrac{\partial\widetilde{A}_1}{\partial y_2}(y_0)\ .
\end{aligned} \tag{7.22}
$$

We observe that by (3.3)

$$
\sin\vartheta(y_0) = -|g|^{-\frac{1}{2}}(y_0)\tilde{H}_3^0/b\ .
$$

So, the study of the constant magnetic field in a half-space done in Section 2, (more precisely (3.10), property 7. in Subsection 3.3 and Theorem 3.11), (7.21) and (7.22) show that there exists $\epsilon_1>0$, such for all $w\in C^\infty(\overline{I\!R_+}^3)$ with compact support,

$$
q^h_{\widetilde{A}^{(1)}}(w) \ge bh\left(\Theta_0+\epsilon_1|g|^{-1/2}(y_0)\frac{|\widetilde{H}_3^0|}{b}\right)|g|^{1/2}(y_0)\int_{I\!R^2\times I\!R_+}|w|^2dy\ , \tag{7.23}
$$

We will consider two cases. Let $C_1>1$ to be chosen later. For more simplicity, we can assume, after a rotation and a dilation in (y_1,y_2), that the metric g is standard at y_0 :

$$
g(y_0) = (\delta_{ij}). \tag{7.24}
$$

First case: $\dfrac{|\widetilde{H}_3^0|}{b} \ge \dfrac{C_1}{\epsilon_1}h^{-1/2}\tau(h)^2$.

We take $k=1$. Then (7.19),(7.20) and (7.23) prove that

$$
\begin{aligned}
&q^h_A(\chi_{\gamma,\tau(h)}u)+C(\tau(h))^2\|\chi_{\gamma,\tau(h)}u\|\cdot(q^h_A(\chi_{\gamma,\tau(h)}u))^{1/2}\\
&\ge [bh(\Theta_0+C_1h^{-1/2}\tau(h)^2)-C(h\tau(h)+(\tau(h))^4)]\cdot\|\chi_{\gamma,\tau(h)}u\|^2\ .
\end{aligned} \tag{7.25}
$$

This implies :

$$
\begin{aligned}
&\left((q^h_A(\chi_{\gamma,\tau(h)}u))^{1/2}+C\tau(h)^2\|\chi_{\gamma,\tau(h)}u\|\right)^2\\
&\quad\ge bh(\Theta_0+C_1h^{-1/2}\tau(h)^2)\cdot(1-C\tau(h))\|\chi_{\gamma,\tau(h)}u\|^2\ .
\end{aligned} \tag{7.26}
$$

Taking the square root, we get :

$$\begin{aligned}&(q_A^h(\chi_{\gamma,\tau(h)}u))^{1/2}\\&\quad\geq\Big((bh)^{\frac{1}{2}}(\Theta_0+C_1h^{-1/2}\tau(h)^2)^{\frac{1}{2}}\cdot(1-C\tau(h))\quad-C\tau(h)^2\Big)\,\|\chi_{\gamma,\tau(h)}u\|\,.\end{aligned}\tag{7.27}$$

This finally gives, if C_1 is large enough and if, for some $\epsilon_0>0$, the weight $\tau(h)$ satisfies the condition $h^{\frac{1}{4}+\epsilon_0}\geq\tau(h)\geq h^{1/2}$,

$$q_A^h(\chi_{\gamma,\tau(h)}u)\geq h\,\left(b(\Theta_0+\frac{1}{2}C_1h^{-1/2}\tau(h)^2)-C\tau(h)\right)\,\|\chi_{\gamma,\tau(h)}u\|^2\,.\tag{7.28}$$

So if $h^{\frac{1}{4}+\epsilon_0}\geq\tau(h)\geq h^{1/2}$ and C_1 is large enough, there exists $h_0>0$ such that

$$q_A^h(\chi_{\gamma,\tau(h)}u)\geq bh\Theta_0\|\chi_{\gamma,\tau(h)}u\|^2,\ \forall h\in]0,h_0]\,.\tag{7.29}$$

We now keep C_1 fixed such that (7.29) is satisfied.

Second case: $\dfrac{|\widetilde{H}_3^0|}{b}<\dfrac{C_1}{\epsilon_1}\,h^{-1/2}\tau(h)^2$.

We proceed by steps :

Step1: We use (7.21) but we take $k=2$. This leads to :

$$\begin{aligned}q_A^h(\chi_{\gamma,\tau(h)}u)\quad&\geq(1-C\tau(h))q^h_{\widetilde{A}^{(k)}}(\chi_{\gamma,\tau(h)}u)\\&\quad-C(\tau(h))^3\|\chi_{\gamma,\tau(h)}u\|\cdot(q_A^h(\chi_{\gamma,\tau(h)}u))^{1/2}\\&\quad-C(\tau(h))^4\|\chi_{\gamma,\tau(h)}u\|^2\,,\end{aligned}\tag{7.30}$$

Step 2: Let us now remark that

$$\begin{aligned}q^h_{\widetilde{A}^{(2)}}(\chi_{\gamma,\tau(h)}u)\quad&\geq q^h_{\widetilde{A}^{(2,1)}}(\chi_{\gamma,\tau(h)}u)\\&\quad-C[\tau(h)\|y_3\chi_{\gamma,\tau(h)}u\|+\|y_3^2\chi_{\gamma,\tau(h)}u\|]\cdot(q_A^h(\chi_{\gamma,\tau(h)}u))^{1/2}\\&\quad-C[\tau(h)^2\|y_3\chi_{\gamma,\tau(h)}u\|^2+\|y_3^2\chi_{\gamma,\tau(h)}u\|^2]\,,\end{aligned}\tag{7.31}$$

with

$$\begin{aligned}&\widetilde{A}^{(2,1)}=\widetilde{A}(y_0)+\textstyle\sum_{j=1}^3(y_j-y_{0j})\frac{\partial\widetilde{A}}{\partial y_j}(y_0)\\&+\textstyle\sum_{j=1}^2(y_j-y_{0j})^2\frac{\partial^2\widetilde{A}}{\partial y_j^2}(y_0)+2(y_1-y_{01})(y_2-y_{02})\frac{\partial^2\widetilde{A}}{\partial y_1\partial y_2}(y_0)\,.\end{aligned}\tag{7.32}$$

Step 3: But it is easy to find a real polynomial function $p(y)$ such that

$$q^h_{\widetilde{A}^{(2,1)}}(\chi_{\gamma,\tau(h)}u)=q^h_{\widetilde{A}^{(2,1,0)}}(e^{i\frac{p}{h}}\chi_{\gamma,\tau(h)}u)\tag{7.33}$$

with

$$\begin{aligned}\widetilde{A}_1^{(2,1,0)}&=\widetilde{H}_2^0y_3+a_1y_2^2+b_1(y),\\\widetilde{A}_2^{(2,1,0)}&=-\widetilde{H}_1^0y_3+\widetilde{H}_3^0y_1+a_2y_1^2+b_2(y),\\\widetilde{A}_3^{(2,1,0)}&=0\,,\end{aligned}\tag{7.34}$$

where :

$$b_1(y)=c_{11}\ y_1y_3+c_{12}\ y_2y_3\ ,\ b_2(y)=c_{21}\ y_1y_3+c_{22}\ y_2y_3\ .$$

Step 4: Modulo an error like in the right hand side of (7.31), we are reduced to the analysis of

$$\begin{array}{ll} \widetilde{A}_1^{(2,1,1)} & = \widetilde{H}_2^0 y_3 + a_1 y_2^2, \\ \widetilde{A}_2^{(2,1,1)} & = -\widetilde{H}_1^0 y_3 + \widetilde{H}_3^0 y_1 + a_2 y_1^2, \\ \widetilde{A}_3^{(2,1,1)} & = 0\,. \end{array} \tag{7.35}$$

We write

$$\begin{array}{ll} q^h_{\widetilde{A}^{(2,1,1)}}(w) & = h^2 \|D_{y_3} w\|^2 \\ & \quad + \tilde{b}^2 \| \left(y_3 - \tilde{b}^{-1}(\sin\theta L_1 - \cos\theta L_2) \right) w\|^2 \\ & \quad + \|(\cos\theta L_1 + \sin\theta L_2) w\|^2\,, \end{array} \tag{7.36}$$

with

$$\begin{array}{ll} \tilde{b} & = [(\widetilde{H}_1^0)^2 + (\widetilde{H}_2^0)^2]^{1/2}\,, \\ \widetilde{H}_1^0 & = \tilde{b}\cos\theta, \\ \widetilde{H}_2^0 & = \tilde{b}\sin\theta, \end{array}$$

and

$$L_1 = hD_{y_1} - a_1 y_2^2, \quad L_2 = hD_{y_2} - \widetilde{H}_3^0 y_1 - a_2 y_1^2\,. \tag{7.37}$$

As the operator $\sin\theta L_1 - \cos\theta L_2$, a priori defined on $\mathcal{S}(I\!R^2)$, has a self-adjoint realization on $L^2(I\!R^2)$. This is indeed, after rotation, an operator of the form $\frac{1}{i}\partial_t + \phi(t,y)$ which is unitary equivalent to $\frac{1}{i}\partial_t$. Hence, we can consider the spectral representation of $\sin\theta L_1 - \cos\theta L_2$ and the analysis of Subsection 2.1 to see that

$$h^2\|D_{y_3} w\|^2 + \tilde{b}^2 \|(y_3 - \tilde{b}^{-1}(\sin\theta L_1 - \cos\theta L_2))w\|^2 \geq h\tilde{b}\Theta_0 \|w\|^2\,. \tag{7.38}$$

Step 5: We now compare b and $\tilde{b}$. We are in the case when $\frac{|\widetilde{H}_3^0|}{b} < C_1 h^{-1/2}\tau(h)^2$. So

$$|b - \tilde{b}| \leq C\, C_1^2 h^{-1}\tau(h)^4\,. \tag{7.39}$$

Step 6: Then (7.30), (7.24) and (7.31) - - (7.39) prove that, if u^h is the eigenfunction associated to the ground state energy of $P^{h,N}_{A,\Omega}$ and if $\tau(h) = h^{1/3}$, then

$$\begin{array}{ll} q^h_A(\chi_{\gamma,\tau(h)} u^h) & \geq [hb\Theta_0 - Ch^{4/3}] \|\chi_{\gamma,\tau(h)} u^h\|^2 \\ & \quad - Ch^{\frac{2}{3}} ||t\chi_{\gamma,\tau(h)} u^h||^2 - C||t^2 \chi_{\gamma,\tau(h)} u^h||^2 \\ & \quad - Ch^{\frac{1}{3}} ||t\chi_{\gamma,\tau(h)} u^h|| \left[q^h_A(\chi_{\gamma,\tau(h)} u^h)\right]^{\frac{1}{2}} \\ & \quad - C\, ||t^2 \chi_{\gamma,\tau(h)} u^h|| \left[q^h_A(\chi_{\gamma,\tau(h)} u^h)\right]^{\frac{1}{2}}\,. \end{array} \tag{7.40}$$

We now eliminate the two last lines at the price of a worst error term. We get first the existence of C such that :

$$\begin{array}{ll} (1 + Ch^{\frac{1}{3}})\, q^h_A(\chi_{\gamma,\tau(h)} u^h) & \geq \left(hb\Theta_0 - Ch^{4/3}\right) \|\chi_{\gamma,\tau(h)} u^h\|^2 \\ & \quad - Ch^{\frac{1}{3}} ||t\chi_{\gamma,\tau(h)} u^h||^2 - Ch^{-\frac{1}{3}} ||t^2 \chi_{\gamma,\tau(h)} u^h||^2\,, \end{array} \tag{7.41}$$

which leads to the existence of C such that :

$$\begin{aligned} q_A^h(\chi_{\gamma,\tau(h)}u^h) \quad &\geq \left(hb\Theta_0 - Ch^{4/3}\right)\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ &\quad -Ch^{\frac{1}{3}}||t\chi_{\gamma,\tau(h)}u^h||^2 - Ch^{-\frac{1}{3}}||t^2\chi_{\gamma,\tau(h)}u^h||^2 \ . \end{aligned} \tag{7.42}$$

The two last terms will be controlled by summation using Proposition 7.1.

End of the proof .
With $\tau(h) = h^{1/3}$, we get from (7.29) and (7.42) that

$$\begin{aligned} q_A^h(\chi_{\gamma,\tau(h)}u^h) \quad &\geq [b\Theta_0 h - C\,h^{4/3}]\cdot\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ &\quad -Ch^{\frac{1}{3}}||t\chi_{\gamma,\tau(h)}u^h||^2 - Ch^{-\frac{1}{3}}||t^2\chi_{\gamma,\tau(h)}u^h||^2 \ , \end{aligned} \tag{7.43}$$

if $\gamma \in \Gamma^1_{\tau(h)}(\Omega)$.
Using Proposition 7.1, we verify that :

$$\sum_{\gamma\in\Gamma^1_{\tau(h)}} \left(h^{\frac{1}{3}}||t\chi_{\gamma,\tau(h)}u^h||^2 + h^{-\frac{1}{3}}||t^2\chi_{\gamma,\tau(h)}u^h||^2\right) \leq Ch^{\frac{4}{3}} \ . \tag{7.44}$$

So we get

$$\sum_{\gamma\in\Gamma^1_{\tau(h)}} q_A^h(\chi_{\gamma,\tau(h)}u^h) \geq (b\Theta_0 h)\cdot\sum_{\gamma\in\Gamma^1_{\tau(h)}}\|\chi_{\gamma,\tau(h)}u^h\|^2 \ - \ C\,h^{4/3}||u_h||^2 \ . \tag{7.45}$$

Then (7.17) is deduced from (7.13) - - (7.16) with $\tau(h) = h^{1/3}$, (7.18) and from (7.45).

8 Refined adapted coordinates on the boundary

8.1 Curvatures

For the following geometric properties of embedded surface in $\mathbb{R}^3$, we refer mainly to the first chapter of [DHKW] (see also the volume two of Spivak's book [Sp]). Let us suppose more specifically that x_0 is a point of the boundary $\partial\Omega$. The neighborhood of x_0 $\mathcal{V}_{x_0}$ can be chosen such that, in $W_{x_0} := \partial\Omega \cap \mathcal{V}_{x_0}$, there exist local coordinates (y_1, y_2), i.e. there exists an open subset $\mathcal{S}$ of $\mathbb{R}^2$ and a diffeomorphism

$$\phi \ : \ \partial\Omega\cap\mathcal{V}_{x_0} \ \to \ \mathcal{S}, \quad \phi(x) = (y_1, y_2). \tag{8.1}$$

We denote by $y \mapsto x(y)$ its inverse. Then $\{\frac{\partial x}{\partial y_1}, \ \frac{\partial x}{\partial y_2}\}$ is a basis of $T\mathcal{W}_{x_0}$.
The first fundamental form of $\partial\Omega$ is the restriction of g_0 to $\partial\Omega$ and it is denoted by G. In the local coordinates (y_1, y_2), G is given by :

$$G = \sum_{1\leq i,j\leq 2} G_{ij}dy_i\otimes dy_j, \quad G_{ij} = \sum_{k=1}^{3}\frac{\partial x_k}{\partial y_i}\cdot\frac{\partial x_k}{\partial y_j}. \tag{8.2}$$

The element of area is given by

$$ds^2 = |G|^{\frac{1}{2}} dy_1 \wedge dy_2,$$

with

$$|G| = \det(G_{ij})_{1 \leq i,j \leq 2}),$$

The unit normal vector to $\partial\Omega$ is defined by

$$N = \frac{\frac{\partial x}{\partial y_1} \wedge \frac{\partial x}{\partial y_2}}{|\frac{\partial x}{\partial y_1} \wedge \frac{\partial x}{\partial y_2}|} \, . \tag{8.3}$$

For any vector fields X and Y, $X \wedge Y$ is the vector field defined by

$$\begin{array}{l} \omega_3(X, Y, X \wedge Y) = |X|^2 \cdot |Y|^2 - (< X, Y >)^2 \, , \\ < X | X \wedge Y > = < Y | X \wedge Y > = 0 \, . \end{array} \tag{8.4}$$

When $\partial\Omega$ is the boundary of a bounded regular domain, we can choose moreover these coordinates such that N is the interior normal unit vector, and we observe, using (8.4), that :

$$\omega_3(\frac{\partial x}{\partial y_1}, \frac{\partial x}{\partial y_2}, N) > 0 \, .$$

Remembering that $|N|^2 = 1$, we get that, for $j = 1, \ 2$,

$$\frac{\partial N}{\partial y_j} \ \in \ T\partial\Omega \, .$$

This permits us to introduce the Weingarten map k from $T\partial\Omega$ into $T\partial\Omega$, by :

$$k(\sum_{j=1}^{2} \lambda_j \frac{\partial x}{\partial y_j}) = - \sum_{j=1}^{2} \lambda_j \frac{\partial N}{\partial y_j} \, .$$

This map is independent of the choice of the coordinates respecting (8.3) with N inner normal.
The second fundamental form K on $T\partial\Omega$ is defined, for X and Y in $T\partial\Omega$, by

$$K(X, Y) = G(X, k(Y)) = \sum_{1 \leq i,j \leq j} K_{ij} \ X_i \, Y_j \, , \tag{8.5}$$

where

$$K_{ij} = - < \frac{\partial x}{\partial y_i} | \frac{\partial N}{\partial y_j} >, \tag{8.6}$$

and X_j and Y_j are the components of X and Y in the local basis $(\frac{\partial}{\partial y_j})$.
Observing that $< \frac{\partial x}{\partial y_i} | N >= 0$, it is easy to see, by differentiating this equality, that

$$K_{ij} = < \frac{\partial^2 x}{\partial y_i \partial y_j} | N > \ . \tag{8.7}$$

In particular K is symmetric. We recall that the Gauss curvature is

$$\kappa^G = \det(k) = (K_{11}K_{22} - K_{12}^2)/(G_{11}G_{22} - G_{12}^2), \tag{8.8}$$

and that the mean curvature is

$$\kappa^M = \frac{1}{2}\mathrm{tr}(k) = \frac{1}{2}(k_{11} + k_{22}), \tag{8.9}$$

where $(k_{ij})_{ij}$ is the matrix $G^{-1}K$.
Let $a > 0$. If $[-a, +a] \ni t \mapsto \gamma(t) \in \partial\Omega$ defines a parametrized curve, we denote its image by Γ. We assume moreover that it is parametrized by arc length, that is :

$$|\gamma'(\tau)| = 1 \ . \tag{8.10}$$

The curvature vector (κ_g, κ_n) of Γ is defined[4] by

$$\frac{d^2\gamma}{d\tau^2}(\tau) = -\kappa_g(\tau)\, N(\gamma(\tau)) \wedge \gamma'(\tau) \ + \ \kappa_n(\tau)\, N(\gamma(\tau)) \ . \tag{8.11}$$

The function κ_g is called the geodesic curvature and κ_n the normal curvature of Γ, at the point $\gamma(\tau)$.
As shown in [DHKW] (Formula (18)), the normal curvature is given by the equation

$$\kappa_n(\tau) = K(\gamma'(\tau), \gamma'(\tau)) \ . \tag{8.12}$$

Remark 8.1 .
Note (cf [DHKW]) that the geodesic curvature vanishes when γ is a geodesic. Let us also recall that the scalar curvature of Γ is

$$\kappa = \mid \frac{d^2\gamma}{d\tau^2} \mid = (\kappa_g^2 + \kappa_n^2)^{\frac{1}{2}} \ .$$

Example 8.2 *The ellipsoid.*
Let us consider the case of the ellipsoid :

$$a_1x_1^2 + a_2x_2^2 + a_3x_3^2 = 1 \ .$$

Let us compute K in the case when one can parametrize by the two first coordinates and let us consider the case when $x_3 > 0$. So we have :

$$x_1 = y_1 \ , \ x_2 = y_2 \ , \ x_3 = \frac{1}{\sqrt{a_3}}\sqrt{1 - a_1y_1^2 - a_2y_2^2} \ .$$

The interior normal is given by :

$$N = -\frac{1}{\nu}\begin{pmatrix} a_1y_1 \\ a_2y_2 \\ a_3x_3(y_1, y_2) \end{pmatrix} \ ,$$

[4]The definition of the geodesic curvature is not uniform in the literature. Some authors ([DHKW]) use the opposite sign.

where :

$$\nu = \sqrt{a_1^2 y_1^2 + a_2^2 y_2^2 + a_3^2 x_3^2}\ .$$

We can now compute K in these coordinates. We first observe that :

$$\partial N/\partial y_1 = c_1 N - \frac{1}{\nu} \begin{pmatrix} a_1 \\ 0 \\ a_3 \frac{\partial x_3}{\partial y_1} \end{pmatrix}\ ,$$

and

$$\partial N/\partial y_2 = c_2 N - \frac{1}{\nu} \begin{pmatrix} 0 \\ a_2 \\ a_3 \frac{\partial x_3}{\partial y_2} \end{pmatrix}\ .$$

We use the notation $\partial_j = \frac{\partial}{\partial y_j}$. This leads to :

$$\begin{array}{lll} K_{11} & = -\langle \partial_1 N\,,\, \partial_1 x \rangle & = \frac{1}{\nu} a_1 + \frac{1}{\nu} a_3 |\partial_1 x_3|^2 \\ K_{22} & = -\langle \partial_2 N\,,\, \partial_2 x \rangle & = \frac{1}{\nu} a_2 + \frac{1}{\nu} a_3 |\partial_2 x_3|^2 \\ K_{12} & = -\langle \partial_1 N\,,\, \partial_2 x \rangle & = \frac{1}{\nu} a_3 (\partial_1 x_3)(\partial_2 x_3)\ . \end{array}$$

We immediately verify the strict positivity of K. We note indeed that :

$$\begin{array}{ll} K(u\,,\,u) & = \frac{1}{\nu} \left(a_1 u_1^2 + a_2 u_2^2 + a_3 ((\partial_1 x_3)\, u_1 + (\partial_2 x_3)\, u_2)^2 \right) \\ & \geq a_1 u_1^2 + a_2 u_2^2\ . \end{array}$$

Similarly, we have

$$G(u\,,\,u) \quad = \left(u_1^2 + u_2^2 + ((\partial_1 x_3)\, u_1 + (\partial_2 x_3)\, u_2)^2 \right)\ .$$

This leads to the following expression for the Gauss curvature :

$$\kappa^G = \det k = \frac{a_1 a_2 a_3}{\nu^4} = \frac{a_1 a_2 a_3}{(a_1^2 x_1^2 + a_2^2 x_2^2 + a_3^2 x_3^2)^2}\ .$$

8.2 Local coordinates near a curve inside the boundary

Let Γ be a curve in $\partial\Omega$ parametrized by arc lengths on some interval I ($I = [-a, +a]$) : $\Gamma = \{\gamma(s);\ s \in I\}$. So we have $|\gamma'(s)| = 1$. Then, there exists a neighborhood $\mathcal{W}_{x_0}$ of $x_0 = \gamma(0)$ in $\partial\Omega$, such that, for any $z \in \mathcal{W}_{x_0} \cap \Gamma$, there exists a unique geodesic Λ_z through z and normal to Γ. The neighborhood $\mathcal{W}_{x_0}$ of x_0 can also be choosen such that

$$\forall\ x \in \mathcal{W}_{x_0},\ \exists!\ z = z(x) \in \Gamma \cap \mathcal{W}_{x_0}\ s.t.\ d_{\partial\Omega}(x, z) = d_{\partial\Omega}(x, \Gamma)\ , \qquad (8.13)$$

where $d_{\partial\Omega}(\ .\ ,\ .\ )$ denotes the distance on $\partial\Omega$.

Then, there exists an open set S of $\mathbb{R}^2$ and a regular diffeomorphism

$$\phi :\ \mathcal{W}_{x_0} \ \to\ S,\ \phi(x) = (r, s) \text{ with } \pm\, r = d_{\partial\Omega}(x, \Gamma) = d_{\partial\Omega}(x, \gamma(s))\ . \qquad (8.14)$$

We observe that :

$$x(0,s) = \gamma(s)\ .$$

We choose a positive orientation (and this determines the choice of the sign of r), by imposing :

$$\frac{\partial x}{\partial r}(0,s) \wedge \frac{\partial x}{\partial s}(0,s) = N(\gamma(s)), \tag{8.15}$$

where $N(x)$ is the interior normal of $\partial\Omega$ at the point $x \in \partial\Omega$. Then (r,s) are local coordinates in $\mathcal{W}_{x_0}$ and observing that, for any fixed s, $r \mapsto x(r,s)$ is a parametrization by arc lengths of the geodesic $\Lambda_{\gamma(s)}$, we have

$$|\frac{\partial x}{\partial r}(r,s)| = 1\ , \tag{8.16}$$

and

$$< \frac{\partial x}{\partial r}(0,s)|\frac{\partial x}{\partial s}(0,s) >= 0\ . \tag{8.17}$$

More precisely we have the following Lemma.

Lemma 8.3 .
In the above local coordinates, the metric G on $\partial\Omega$ is diagonal :

$$G = dr \otimes dr + \alpha(r,s)\, ds \otimes ds. \tag{8.18}$$

On the curve Γ, we have

$$\alpha(0,s) = 1,\ \frac{\partial \alpha}{\partial r}(0,s) = -2\kappa_g(s) \text{ and } \frac{\partial \alpha}{\partial s}(0,s) = 0\ . \tag{8.19}$$

where $\kappa_g(s)$ denotes geodesic curvature of the curve Γ at $\gamma(s)$.

Proof.
As for any fixed s, the map $r \mapsto x(r,s)$ is a parametrization by arc lengths of the geodesic $\Lambda_{\gamma(s)}$, the curvature of $\Lambda_{\gamma(s)}$ is given, using (8.11), (8.12) and Remark 8.1, by

$$\frac{\partial^2 x}{\partial r^2}(r,s) = K(\frac{\partial x}{\partial r}(r,s), \frac{\partial x}{\partial r}(r,s))\, N(x(r,s))\ . \tag{8.20}$$

Then, we get from (8.20) that

$$\frac{\partial}{\partial r} < \frac{\partial x}{\partial s}|\frac{\partial x}{\partial r} >=< \frac{\partial^2 x}{\partial s \partial r}|\frac{\partial x}{\partial r} >= \frac{1}{2}\frac{\partial}{\partial s} < \frac{\partial x}{\partial r}|\frac{\partial x}{\partial r} >\ . \tag{8.21}$$

So, using in addition (8.16), we have

$$\frac{\partial}{\partial r} < \frac{\partial x}{\partial s}|\frac{\partial x}{\partial r} >= 0\ . \tag{8.22}$$

But $\Lambda_{\gamma(s)}$ is normal to Γ; so $< \frac{\partial x}{\partial s}(0,s)|\frac{\partial x}{\partial r}(0,s) >= 0$. Then, using (8.22), we get :

$$< \frac{\partial x}{\partial s}(r,s)|\frac{\partial x}{\partial r}(r,s) >= 0\ . \tag{8.23}$$

This shows that the metric is diagonal as announced in (8.18) with

$$\alpha(r,s) = < \frac{\partial x}{\partial s}(r,s) | \frac{\partial x}{\partial s}(r,s) > \ .$$

We get also from the orthogonality of γ' and γ'' that

$$\frac{\partial \alpha}{\partial s}(0,s) = 0 \ .$$

But, differentiating the identity (8.23) with respect to s, we have

$$\frac{\partial \alpha}{\partial r}(r,s) = 2 < \frac{\partial^2 x}{\partial s \partial r} | \frac{\partial x}{\partial s} > = -2 < \frac{\partial x}{\partial r} | \frac{\partial^2 x}{\partial s^2} > . \tag{8.24}$$

But, by (8.11), we have :

$$\frac{\partial^2 x}{\partial s^2}(0,s) = \kappa_n(\gamma(s))N(\gamma(s)) + \kappa_g(\gamma(s))\frac{\partial x}{\partial s}(0,s) \wedge N(\gamma(s)) \ ,$$

so (8.15) and (8.17) lead to

$$\frac{\partial^2 x}{\partial s^2}(0,s) = \kappa_n(\gamma(s))N(\gamma(s)) + \kappa_g(\gamma(s))\frac{\partial x}{\partial r}(0,s). \tag{8.25}$$

The formulas (8.24) and (8.25) give the non-obvious part of (8.19)

$$\frac{\partial \alpha}{\partial r}(0,s) = -2\kappa_g(\gamma(s)) \ .$$

Remark 8.4 .
In the coordinates (r,s) introduced in Lemma 8.3, the second fondamental form is given (see (8.7))

$$K = K_{11}\ dr \otimes dr \ + \ K_{12} dr \otimes ds \ + \ K_{21}\ ds \otimes dr \ + \ K_{22}\ ds \otimes ds \ ,$$

is given by

$$\begin{array}{ll} K_{11}(r,s) & = < \frac{\partial^2 x}{\partial r^2}(r,s) | N(x(r,s)) >, \\ K_{22}(r,s) & = < \frac{\partial^2 x}{\partial s^2}(r,s) | N(x(r,s)) >, \\ K_{12}(r,s) & = < \frac{\partial^2 x}{\partial r \partial s}(r,s) | N(x(r,s)) > \\ K_{21}(r,s) & = K_{12}(r,s) \ . \end{array}$$

The function $K_{11}(r,s)$ is the normal curvature of the geodesic $\Lambda_{\gamma(s)}$ at $x(r,s)$ and the function $K_{22}(0,s) = \kappa_n(\gamma(s))$ is the normal curvature of the curve Γ at $x(0,s) = \gamma(s)$.

8.3 Local coordinates near a curve in the boundary

We come back to previous computations and relate them to the curvatures. Let $\phi(x) = (y_1, y_2)$ be local coordinates of the boundary as defined in (8.1). We have observed in (5.19), that

$$g_0 = dy_3 \otimes dy_3 + \sum_{1 \le i,j \le 2} [G_{ij}(y_1,y_2) - 2y_3 K_{ij}(y_1,y_2) + y_3^2 L_{ij}] dy_i \otimes dy_j \ , \tag{8.26}$$

where

- $G = \sum_{1\leq i,j\leq 2} G_{ij}\, dy_i \otimes dy_j$,
- $K = \sum_{1\leq i,j\leq 2} K_{ij}\, dy_i \otimes dy_j$,
- $L = \sum_{1\leq i,j\leq 2} L_{ij}\, dy_i \otimes dy_j = \sum_{1\leq i,j\leq 2} < \frac{\partial N}{\partial y_i} | \frac{\partial N}{\partial y_j} > dy_i \otimes dy_j$.

G, K and L are respectively called the first, second and third fundamental forms on $\partial\Omega$. If we take local coordinates $(y_1, y_2) = (r, s)$ on the boundary given by Lemma 8.3, the sesquilinear form introduced in (5.15) becomes

$$\begin{array}{l} q_A^h(u) \\ = \int_{\mathcal{V}_{x_0}} |g|^{\frac{1}{2}} [|hD_{y_3} - \widetilde{A}_3 u|^2 \ + \sum_{1\leq i,j\leq 2} g^{ij} (hD_{y_i} u - \widetilde{A}_i u) \cdot \overline{(hD_{y_j} u - \widetilde{A}_j u)}]\, dy^3, \end{array} \tag{8.27}$$

for u supported in $\mathcal{V}_{x_0}$, the associated differential operator is

$$\begin{array}{rl} P_A^h & = (hD_{y_3} - \widetilde{A}_3)^2 + \frac{h}{2i} |g|^{-1} (\frac{\partial}{\partial y_3} |g|)(hD_{y_3} - \widetilde{A}_3) \\ & \quad + |g|^{-\frac{1}{2}} \sum_{1\leq i,j\leq 2} (hD_{y_j} - \widetilde{A}_j)(|g|^{\frac{1}{2}} g^{ij} (hD_{y_i} - \widetilde{A}_i))\ . \end{array} \tag{8.28}$$

If we now consider the coordinates introduced in Subsection 8.2, that is $(y_1, y_2) = (s, t)$ and complete by $t = y_3$ introduced in Subsection 5.3, then

$$|g| = \alpha(r, s) - 2t[\alpha(r, s) K_{11}(r, s) + K_{22}(r, s)] + t^2 \epsilon_3(r, s, t), \tag{8.29}$$

and, for $1 \leq i, j \leq 2$,

$$(g^{ij})_{1\leq i,j\leq 2} = \begin{pmatrix} 1 & 0 \\ 0 & \alpha^{-1} \end{pmatrix} + 2t \begin{pmatrix} K_{11} & \alpha^{-1} K_{12} \\ \alpha^{-1} K_{21} & \alpha^{-2} K_{22} \end{pmatrix} + t^2 R\ , \tag{8.30}$$

where ϵ_3 and R_{ij} are smooth functions.

8.4 More magnetic geometry

We assume that the magnetic field $H = \operatorname{curl} A$ is constant and we can assume, without loss of generality, that :

$$A(x) = \frac{b}{2}(0, -x_3, x_2) \tag{8.31}$$

for some fixed $b > 0$.
Let Ω be bounded open set of $I\!R^3$ with regular boundary $\partial\Omega$. We now assume that (1.5) is satisfied.

Remark 8.5 .
We observe that this assumption is satisfied when Ω is strictly convex.

In this situation, we can introduce the following definition :

Definition 8.6 .
At each point x of Γ, we introduce the normal curvature along the magnetic field $H = V(B)$ by :

$$\kappa_{n,B}(x) := K_x(\gamma' \wedge N \ , \ \frac{H}{|H|}) \ , \tag{8.32}$$

where K denotes the second fundamental form on the surface $\partial\Omega$.

We have already introduced $\kappa_{n,B}$ in (8.32). Similarly, we can define :

$$\kappa_{t,B}(s) = K(\gamma'(s), \frac{V(B)}{|V(B)|}) \ . \tag{8.33}$$

We observe that we have :

$$\begin{array}{ll} \kappa_{n,B}(s) & = K(\frac{\partial}{\partial r}, \frac{V(B)}{|V(B)|}) = \cos\theta(s) K_{11}(0,s) + \sin\theta(s) K_{12}(0,s) \ ; \\ \kappa_{t,B}(s) & = K(\frac{\partial}{\partial s}, \frac{V(B)}{|V(B)|}) = \cos\theta(s) K_{12}(0,s) + \sin\theta(s) K_{22}(0,s) \ . \end{array} \tag{8.34}$$

Let us observe that the angle $\theta(s)$ is not "free" in our picture. We can indeed, by computing $V(B)$ in the new coordinates (and remembering (5.5) and Lemma 8.3), get the relation :

$$(b\cos\theta(s))^2 + (1 - 2\kappa_g(s) r)[b\sin\theta(s) + rb(2\kappa_g(s) - \theta'(s))\sin\theta(s)]^2 + \mathcal{O}(r^2) = b^2 \ .$$

Looking at the coefficient of r, we get

$$\kappa_g(s) = \theta'(s) \ , \tag{8.35}$$

or

$$\theta(s) = 0 \ . \tag{8.36}$$

The case θ constant corresponds to the case when γ is a geodesic. In fact we have the geometrical fact:

Proposition 8.7 .
The assumption $V(B)$ is constant (of norm equal to one) and tangent to the surface $\partial\Omega$ along the curve Γ implies that

$$\kappa_{t,B}(x) = 0, \quad \forall \ x \ \in \ \Gamma \ . \tag{8.37}$$

If $s \mapsto \gamma(s)$ is a parametrization of Γ by arc length, with

$$\theta(s) = \ \text{Arcsin} \ ((\gamma'(s), V(B)))$$

then

$$\theta'(s) = \kappa_g(\gamma(s)), \quad \forall \ s \ . \tag{8.38}$$

Proof of Proposition 8.7.
Let us write :

$$V(B) = \sin(\theta(s))\gamma'(s) + \cos(\theta(s))[\gamma'(s) \wedge N(\gamma(s)] \ , \tag{8.39}$$

As $V(B)$ is constant, we can differentiate with respect to s (8.39) and we get :

$$\begin{aligned}
&\theta'(s)\,[\cos(\theta(s))\gamma'(s) - \sin(\theta(s))\gamma'(s) \wedge N(\gamma(s))] \\
&+ \sin(\theta(s))\gamma''(s) \\
&+ \cos(\theta(s))\,[\gamma''(s) \wedge N(\gamma(s)) + \gamma'(s) \wedge (N \circ \gamma)'(s)] \\
&= 0\,.
\end{aligned}$$

But using the coordinates of Lemma 8.3, the formula (8.6) proves

$$(N \circ \gamma)' = -K_{12}(\gamma)\gamma' \wedge N(\gamma) - K_{22}(\gamma)\gamma'\,,$$

and (8.25) becomes

$$\gamma'' = \kappa_g(\gamma)\gamma' \wedge N(\gamma) + \kappa_n(\gamma)N(\gamma)$$

So

$$\begin{aligned}
&\theta'[\cos\theta\,\gamma' - \sin\theta\,\gamma' \wedge N(\gamma)] \\
&+ \sin\theta\,[\kappa_g(\gamma)\gamma' \wedge N(\gamma) + \kappa_n(\gamma)N(\gamma)] \\
&+ \cos\theta\,[-\kappa_g(\gamma)\gamma' + K_{12}(\gamma)N(\gamma)] \\
&= 0\,,
\end{aligned}$$

and then, expressing the previous equality on the basis $\gamma' \wedge N$, γ', N,

$$\begin{aligned}
\cos\theta\,[\theta' - \kappa_g(\gamma)] &= 0 \\
\sin\theta\,[-\theta' + \kappa_g(\gamma)] &= 0 \\
\sin\theta\,\kappa_n(\gamma) + \cos\theta\,K_{12}(\gamma) &= 0\,.
\end{aligned} \tag{8.40}$$

We get (8.38), and using (8.12) we get also (8.37) from $\kappa_n(\gamma) = K_{22}(\gamma)$ and from (8.34).

Remark 8.8 .
In the case when $\partial\Omega$ is strictly convex, ($K > 0$), then (8.37) implies that

$$\kappa_{n,B} \neq\ 0,\ \forall\, x\ \in\ \Gamma\,. \tag{8.41}$$

One can also meet degenerate cases where K is not invertible (locally cylindric domains).
When $\theta(s) = 0$, we deduce from (8.34) and (8.37) that $K_{12}(x(s)) = 0$. So the curvature matrix K becomes diagonal.

Proof of Remark 8.8.
We observe that (8.34) can be rewritten in the form :

$$\begin{pmatrix} \kappa_{n,B} \\ \kappa_{t,B} \end{pmatrix} = K \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \tag{8.42}$$

Observing that K is inversible when Ω is strictly convex (K is actually strictly positive), we immediately see that $|\kappa_{n,B}| + |\kappa_{t,B}| \neq 0$.

Remark 8.9 .
The condition that $\theta' = \kappa_g$ is obtained also in the case $\theta \equiv 0$. So in this case we have effectively $\kappa_g = 0$. So Γ should be a geodesic. Conversely, when Γ is a geodesic, we should have $\theta \equiv 0$ if $V(B)$ is constant. We observe indeed that by computing the circulation of $V(B)$ along Γ and using Stokes Lemma (or more simply that $V(B) \cdot \gamma' = \frac{d}{dt}(V(B) \cdot \gamma)$), we should have :

$$\int_\Gamma \sin\theta(s) ds = 0 \ .$$

When θ is constant, this implies $\theta = 0$.

Example 8.10 .
In the case of the ellipsoid considered in Example 8.2, it is interesting to compute our invariants. Take for simplification, the case when $B = (0, 0, 1)$. Then Γ is the intersection of the ellipsoid with $x_3 = 0$. So we get an ellipse in this plane. We can now observe that the condition (9.2) is satisfied. The vector field H is orthogonal to Γ. We observe that :

$$\langle H \ , \ N \rangle = -|B| \frac{a_3 x_3}{\nu} \ .$$

This leads to :

$$|\kappa_{n,B}(y_1, y_2)| = \frac{a_3}{\nu} \ .$$

The minimum of $\kappa_{n,B}$ (which appears in Formula (9.4)) is then obtained at the point where ν is maximal. If we assume for example that $a_1 > a_2$, we get that this maximum is obtained at $x_2 = x_3 = 0$ and equal to a_1. This is not conformed to the intuition we got from the two-dimensional case.

9 Curvature effects on the ground state energy in the case of constant magnetic field: Main statements

Theorem 9.1 .
Let $P_{A,\Omega}^{h,N}$ be the Neumann realization of the magnetic Laplacian $(hD - A)^2$ on $L^2(\Omega)$, where $h \in]0, 1[$ is a small parameter. We assume that (1.5) is satisfied and that :

$$\kappa_{n,B} \neq 0, \forall x \in \ \Gamma \ . \tag{9.1}$$

We assume moreover that :

$$\text{The magnetic field } H \text{ is orthogonal to } \Gamma. \tag{9.2}$$

Then there exists $\eta > 0$ such that :

$$\inf \ \text{Sp} \ (P_{A,\Omega}^{h,N}) = b\Theta_0 h + \hat{\gamma}_0 b^{\frac{2}{3}} h^{\frac{4}{3}} + \mathcal{O}(h^{\eta + \frac{4}{3}}) \ , \tag{9.3}$$

where

$$\hat{\gamma}_0 = \frac{1}{2}\hat{\nu}_0[\mu''(\xi_0)]^{\frac{1}{3}} \inf_{x\in\Gamma} |\kappa_{n,B}(x)|^{\frac{2}{3}}. \tag{9.4}$$

Here the constants Θ_0, ξ_0 and the function $\mu(t)$ are those defined in subsections 2.1 and 2.2. The constant $\hat{\nu}_0$ is defined in Subsection 2.4.

The assumption (8.32) says that the constant magnetic field is tangent exactly at order one on $\partial\Omega$, for any $x \in \Gamma$. We observe indeed, using (8.6) and (8.32), that :

$$\kappa_{n,B} = -\frac{\partial}{\partial r}(\langle N\ ,\ \frac{H}{|H|}\rangle)\ . \tag{9.5}$$

Without the assumption (9.2), we shall only prove :

Theorem 9.2 .
Let $P^{h,N}$ be the Neumann realization on $L^2(\Omega)$ of the magnetic Laplacian $(hD-A)^2$, where $h \in]0,1[$ is a small parameter. We assume that (1.5) is satisfied. Then there exists $\eta > 0$ such that :

$$\inf\ \mathrm{Sp}\ (P^{h,N}) \leq b\Theta_0 h + \hat{\gamma}_0 b^{\frac{2}{3}} h^{\frac{4}{3}} + \mathcal{O}(h^{\eta+\frac{4}{3}})\ , \tag{9.6}$$

where

$$\hat{\gamma}_0 = (\frac{1}{2})\hat{\nu}_0(\mu''(\xi_0))^{\frac{1}{3}} \inf_{x\in\Gamma} \left((\kappa_{n,B}(x)^{\frac{2}{3}} (\frac{1}{2}\mu''(\xi_0)\sin^2\theta(x) + \cos^2\theta(x))^{\frac{1}{3}} \right)\ . \tag{9.7}$$

When $\theta \equiv 0$, we recover the statement of Theorem 9.1. We conjecture that we have equality in the general case.

Remark 9.3 .
The expression in (9.7) can be related more directly to the curvature by using the following formula :

$$\begin{aligned} &\kappa_{n,B}(x)^2(\tfrac{1}{2}\mu''(\xi_0)\sin^2\theta(x) + \cos^2\theta(x)) \\ &\quad = \kappa^G(x)^2\ \left(\kappa_n(x)^2 + \tfrac{1}{2}\mu''(\xi_0)K_x(T(x), T(x)\wedge N(x))\right)\times \\ &\qquad \times \left(\kappa_n(x)^2 + K_x(T(x), T(x)\wedge N(x))\right)^{-2}\ . \end{aligned} \tag{9.8}$$

Here, we recall that, for any $x \in \partial\Omega$, $N(x)$ is the unitary interior nornal vector, $\kappa^G(x)$ is the Gauss curvature and $K_x(\cdot,\cdot)$ is the curvature form, (the second fondamental form). Moreover, if $x \in \Gamma$, $T(x)$ denotes the unit tangent vector with a given orientation on each connected component of Γ and $\kappa_n(x) = K_x(T(x), T(x))$ the normal curvature of Γ at x.

This formula is established using the results of Section 8.

10 Towards the model: new normal forms

In this section, the vector magnetic field $V(B)$ is assumed to be constant, more precisely

$$V(B) = b\frac{\partial}{\partial x_1},\ (b = |V(B)| > 0).$$

The set $\Gamma = \{x \in \partial\Omega;\ V(B) \in T_x(\partial\Omega)\}$ is assumed to be a regular curve.
The angle between the normal to Γ in $T_x\partial\Omega$ and $V(B)$ will be denoted by $\theta(x)$.
We will work near a point of Γ x_0 to be determined and will look after a good approximation of the operator in a small box around x_0.
We consider local coordinates (r, s, t) in a neighborhood $\mathcal{V}_{x_0}$ of x_0, such that (r, s) are the coordinates of Lemma 8.3, and such that $t = t(x) = \text{distance}(x, \Gamma))$.

10.1 Normal form for the magnetic potential

In this subsection we shall show how after a suitable gauge transform, we can arrive to a more tractable model. We assume that the magnetic field is constant.

Lemma 10.1 .
Let $\widetilde{A}$ be the magnetic potential defining $\widetilde{B}$, in the coordinates (r, s, t) defined near $x_0 = (0, s_0, 0)$. Let $\widetilde{A}^{(2)}$ the Taylor expansion to order 2 of $\widetilde{A}$. Then there exists a polynomial function of $y = (r, s - s_0, t)$, $p^0(y)$ such that,

$$\tilde{A}^{(2)} = A^0 + \text{grad}_y p^0 \ , \tag{10.1}$$

with

$$\begin{array}{ll} A_1^0 & = bt[\sin\theta_0 + \kappa_g(x_0)\cos\theta_0\,(s - s_0) - \sin\theta_0\,\kappa^M(x_0)t] \ , \\ A_2^0 & = -bt[\cos\theta_0\ - \kappa_g(x_0)\cos\theta_0\, r - \kappa_g(x_0)\sin\theta_0\,(s - s_0) - \cos\theta_0\,\kappa^M(x_0)t] \\ & \quad -\frac{1}{2}b\kappa_{n,B}(x_0)r^2 \\ A_3^0 & = 0\ . \end{array} \tag{10.2}$$

Proof.
To prove this lemma, we have just to determine the Taylor expansion up to order 1 of the magnetic field in the coordinates $(r, s - s_0, t)$ at the point $(0, s_0, 0)$. Let us first recall that we have assumed that A was given by (8.31). So the corresponding vector $V(B)$ introduced in (5.3) is :

$$V(B) = b\frac{\partial}{\partial x_1}\ .$$

Let us analyze its expression in the new coordinates :

$$V(B) = b\frac{\partial}{\partial x_1} = \widetilde{b}_1\frac{\partial}{\partial r} + \widetilde{b}_2\frac{\partial}{\partial s} + \widetilde{b}_3\frac{\partial}{\partial t}, \tag{10.3}$$

and, by (8.26), (8.18) and (10.3), we get

$$b\frac{\partial x_1}{\partial r} =< V(B)|\frac{\partial}{\partial r} >= \widetilde{b}_1(1 - 2tK_{11}) - 2t\widetilde{b}_2K_{12} + \mathcal{O}(t^2), \tag{10.4}$$

$$b\frac{\partial x_1}{\partial s} =< V(B)|\frac{\partial}{\partial s} >= \widetilde{b}_2(\alpha - 2tK_{22}) - 2t\widetilde{b}_1K_{12} + \mathcal{O}(t^2), \tag{10.5}$$

and

$$b\frac{\partial x_1}{\partial t} =< V(B)|\frac{\partial}{\partial t} >= \widetilde{b}_3. \tag{10.6}$$

Using (8.19), (10.4), (10.5) and Schwarz Lemma for x_1, we get :

$$\frac{\partial \widetilde{b}_1}{\partial s} = \frac{\partial}{\partial r}(\alpha \widetilde{b}_2) = -2\kappa_g \widetilde{b}_2 + \frac{\partial \widetilde{b}_2}{\partial r} \, , \tag{10.7}$$

when $t = r = 0$.
We have :

$$\widetilde{b}_1 = b\cos\theta(s), \quad \widetilde{b}_2 = b\sin\theta(s), \widetilde{b}_3 = 0 \, , \tag{10.8}$$

when $t = r = 0$.
This leads by differentiation with respect to s to :

$$\begin{array}{ll} \frac{\partial \bar{b}_1}{\partial s} & = -b\sin\theta(s)\,\theta'(s) \, , \\ \frac{\partial \bar{b}_2}{\partial s} & = b\cos\theta(s)\,\theta'(s) \, , \\ \frac{\partial \bar{b}_3}{\partial s} & = 0 \, , \end{array} \tag{10.9}$$

when $t = r = 0$. Then we get by coming back to (10.7) that (10.8) leads to :

$$\frac{\partial \widetilde{b}_2}{\partial r} = -b\sin\theta\,\theta' + 2\kappa_g b\,\sin\theta \, . \tag{10.10}$$

Differentiating (10.4) with respect to r, we get for $t = 0$,

$$\frac{\partial \widetilde{b}_1}{\partial r} = b\frac{\partial^2 x_1}{\partial r^2} \, , \tag{10.11}$$

and by (8.19)

$$< \frac{\partial x}{\partial r} | \frac{\partial x}{\partial r} >= 1 \, .$$

So differentiating the last equality, we get :

$$< \frac{\partial x}{\partial r} | \frac{\partial^2 x}{\partial r^2} >= 0$$

But when $t = r = 0$, $\frac{\partial x}{\partial r}$ is normal to Γ, so

$$< \frac{\partial x_1}{\partial r} | \frac{\partial^2 x_1}{\partial r^2} >= 0 \, .$$

This gives finally :

$$\frac{\partial \widetilde{b}_1}{\partial r} = b < \frac{\partial x}{\partial r} | \frac{\partial^2 x}{\partial r^2} >= 0 \, , \tag{10.12}$$

when $t = r = 0$. Let us now use (10.6) to write that

$$\frac{\partial \widetilde{b}_3}{\partial r} = \frac{\partial}{\partial r} < V(B) | N >=< V(B) | \frac{\partial N}{\partial r} > \, ,$$

when $t = 0$.
Then, using also (10.3), (10.8) and (8.6), we obtain :

$$< V(B) | \frac{\partial N}{\partial r} >= b\cos\theta(s) < \frac{\partial}{\partial r} \mid \frac{\partial N}{\partial r} > + b\sin\theta(s) < \frac{\partial}{\partial s} \mid \frac{\partial N}{\partial r} > \, .$$

This leads to

$$\frac{\partial \widetilde{b}_3}{\partial r} = -b\,\cos\theta(s)\,K_{11} - b\sin\theta(s)\,K_{12}\,, \tag{10.13}$$

when $t = r = 0$.
But by (10.4), (10.6) and Schwarz Lemma, we have

$$\frac{\partial \widetilde{b}_3}{\partial r} = \frac{\partial \widetilde{b}_1}{\partial t} - 2\widetilde{b}_1 K_{11} - 2\widetilde{b}_2 K_{12} \tag{10.14}$$

when $t = r = 0$.
So, from (10.13), we get :

$$\frac{\partial \widetilde{b}_1}{\partial t} = b\cos\theta(s) K_{11} + b\sin\theta(s) K_{12}\,, \tag{10.15}$$

when $t = r = 0$.

Once again, Schwarz Lemma, (10.5), and (10.6) lead to

$$\frac{\partial \widetilde{b}_3}{\partial s} = \alpha\frac{\partial \widetilde{b}_2}{\partial t} - 2\widetilde{b}_2 K_{22} - 2\widetilde{b}_1 K_{12} \tag{10.16}$$

when $t = 0$.
Then, (8.19), (10.8) and (10.9) lead to

$$\frac{\partial \widetilde{b}_2}{\partial t} = 2b\cos\theta K_{12} + 2b\sin\theta K_{22}\,, \tag{10.17}$$

when $t = r = 0$.
It remains to determine $\frac{\partial \widetilde{b}_3}{\partial t}$ when $t = r = 0$. Let us denote the magnetic field

$$\widetilde{B} = \widetilde{B}_{23}\,ds \wedge dt + \widetilde{B}_{31}\,dt \wedge dr + \widetilde{B}_{12}\,dr \wedge ds\,.$$

So by (5.11) and using the property that :

$$\frac{\partial \widetilde{B}_{23}}{\partial r} + \frac{\partial \widetilde{B}_{31}}{\partial s} + \frac{\partial \widetilde{B}_{12}}{\partial t} = 0\,,$$

we get from (5.13) that

$$|g|^{\frac{1}{2}}[\frac{\partial \widetilde{b}_1}{\partial r} + \frac{\partial \widetilde{b}_2}{\partial s} + \frac{\partial \widetilde{b}_3}{\partial t}] + \frac{1}{2}|g|^{-\frac{1}{2}}[(\partial_t|g|)\widetilde{b}_3 + (\partial_r|g|)\widetilde{b}_1 + (\partial_s|g|)\widetilde{b}_2] = 0\,, \tag{10.18}$$

Let us now use this formula on $t = r = 0$. Using (10.12), (10.9), we get first :

$$\frac{\partial \widetilde{b}_3}{\partial t} + b\cos\theta(s)\theta'(s) = -\frac{1}{2}|g|^{-1}((\partial_t|g|)\widetilde{b}_3 + (\partial_r|g|)\widetilde{b}_1 + (\partial_s|g|)\widetilde{b}_2)\,,$$

on $t = r = 0$.
We now use (8.29) and Lemma 8.3 (more precisely (8.19)), we obtain, using (10.8) :

$$(\partial_r|g|) = -2\kappa_g(s)\,, \quad \text{when } t = r = 0\,. \tag{10.19}$$

This leads to :

$$\frac{\partial \widetilde{b}_3}{\partial t} = b\,(\kappa_g - \theta')\,\cos\theta \text{ when } \;\; t = r = 0. \tag{10.20}$$

We actually need a more complete expansion of $|g|$. We have :

$$|g| = 1 - 2\kappa_g(s_0)r - 2(K_{11}(0,s_0) + K_{22}(0,s_0))t + \mathcal{O}((t,r,s-s_0)^2)\ . \tag{10.21}$$

We can now establish the Taylor expansion of the magnetic field in the coordinates (r,s,t).

We can now establish the formulas in full generality. For $t = r = 0$, we have, with $\theta = \theta(s_0)$:

$$\begin{array}{ll} \tilde{b}_1 & = b\cos\theta\,, \\ \frac{\partial \tilde{b}_1}{\partial r} & = 0, \\ \frac{\partial \tilde{b}_1}{\partial s} & = -b\sin\theta\,, \\ \frac{\partial \tilde{b}_1}{\partial t} & = b\cos\theta K_{11} + b\sin\theta K_{12}\ ; \end{array} \tag{10.22}$$

$$\begin{array}{ll} \tilde{b}_2 & = b\sin\theta(s)\ , \\ \frac{\partial \tilde{b}_2}{\partial r} & = b(2\kappa_g - \theta')\sin\theta\ , \\ \frac{\partial \tilde{b}_2}{\partial s} & = b\cos\theta\,\theta'\ , \\ \frac{\partial \tilde{b}_2}{\partial t} & = 2b\cos\theta K_{12} + 2b\sin\theta K_{22}\ ; \end{array} \tag{10.23}$$

$$\begin{array}{ll} \tilde{b}_3 & = 0\ , \\ \frac{\partial \tilde{b}_3}{\partial r} & = -b\cos\theta K_{11} - b\sin\theta K_{12}, \\ \frac{\partial \tilde{b}_3}{\partial s} & = 0, \\ \frac{\partial \tilde{b}_3}{\partial t} & = b\cos\theta(\kappa_g - \theta')\ . \end{array} \tag{10.24}$$

Using the Taylor extension (to order 1) of $|g|^{\frac{1}{2}}$,

$$|g|^{\frac{1}{2}} = 1 - \kappa_g(s_0)r - (K_{11}(0,s_0) + K_{22}(0,s_0))t + \mathcal{O}(|(r,s-s_0,t)|)\ ,$$

we obtain the model :

$$\begin{array}{ll} \tilde{b}_1^0 & = b\cos\theta(s_0) - b\sin\theta(s_0)\theta'(s_0)(s-s_0) + (b\cos\theta(s_0)K_{11}(0,s_0) \\ & \quad + b\sin\theta(s_0)K_{22}(0,s_0))t\ , \\ \tilde{b}_2^0 & = b\sin\theta(s_0) - b\cos\theta(s_0)\theta'(s_0)(s-s_0) + b\sin\theta(2\kappa_g - \theta'(s_0))r \\ & \quad + (2b\cos\theta K_{12} + 2b\sin\theta(s_0)K_{22})t\ , \\ \tilde{b}_3^0 & = -(b\cos\theta(s_0)K_{11} + b\sin\theta(s_0)K_{12})r \\ & \quad + b\cos\theta(s_0)(\kappa_g - \theta'(s_0))t\ . \end{array} \tag{10.25}$$

These formulas lead to the introduction of the "model" corresponding magnetic field :

$$\begin{array}{ll} \widetilde{B}_{23}^0 & = b\cos\theta_0 - b\sin\theta_0\,\theta'(s_0)(s-s_0) - b\cos\theta_0\kappa_g r \\ & \quad + b((\cos\theta_0 - 1)K_{11} + (\sin\theta_0 - 1)K_{22})t\ , \\ \widetilde{B}_{31}^0 & = b\sin\theta_0 - b\cos\theta_0\,\theta'(s_0)(s-s_0) + b\sin\theta_0(\kappa_g - \theta')r \\ & \quad + b(2\cos\theta_0 K_{12} + \sin\theta_0 K_{22})t\ , \\ \widetilde{B}_{12}^0 & = -b(\cos\theta_0 K_{11} + \sin\theta_0 K_{12})r + b\cos\theta_0(\kappa_g - \theta'(s_0))t\ , \end{array} \tag{10.26}$$

with $\theta_0 = \theta(s_0)$, $K_{ij} = K_{ij}(0, s_0)$.
This corresponds to the Taylor expansion up to order 1 of $\widetilde{B}$ at the point $(0, s_0, 0)$.

$$\begin{aligned}
\widetilde{b}_1 &= b[\cos(\theta(s_0)) - \theta'(s_0)\sin(\theta(s_0))(s - s_0) + \kappa_{n,B}(x_0)t] \\
&\quad +\mathcal{O}(|y|^2) \\
\widetilde{b}_2 &= b[\sin(\theta(s_0)) + \sin(\theta(s_0))(2\kappa_g(x_0) - \theta'(s_0))r \\
&\quad +\theta'(s_0)\cos(\theta(s_0))(s - s_0) + 2\kappa_{t,B}(x_0)t] \\
&\quad +\mathcal{O}(|y|^2) \\
\widetilde{b}_3 &= b[-\kappa_{n,B}(x_0)r + (\kappa_g(x_0) - \theta'(s_0))\cos(\theta(s_0))t] + \mathcal{O}(|y|^2)
\end{aligned} \tag{10.27}$$

As from (8.29)

$$|g|^{\frac{1}{2}} = 1 - \kappa_g r - 2\kappa^M t + \mathcal{O}(|y|^2)\ ,$$

we get using the relation between the magnetic field and the vector magnetic field given by (5.11) and (5.12)

$$\begin{aligned}
\widetilde{B}_{23} &= b[\cos\theta_0 - \kappa_g(x_0)\cos\theta_0\, r - \theta'(s_0)\sin\theta_0\,(s - s_0)] \\
&\quad +b(\kappa_{n,B}(x_0) - 2\cos\theta_0\,\kappa^M(x_0))t \\
&\quad +\mathcal{O}(|y|^2) \\
\widetilde{B}_{31} &= b[\sin\theta_0 + \sin\theta_0\,(\kappa_g(x_0) - \theta'(s_0))r + \theta'(s_0)\cos(\theta_0)(s - s_0)] \\
&\quad +2bt[\kappa_{t,B}(x_0) - \sin\theta_0\,\kappa^M(x_0)] \\
&\quad +\mathcal{O}(|y|^2) \\
\widetilde{B}_{12} &= b[-\kappa_{n,B}(x_0)r + (\kappa_g(x_0) - \theta'(s_0))\cos\theta_0\, t] \\
&\quad +\mathcal{O}(|y|^2)
\end{aligned} \tag{10.28}$$

with $\theta_0 := \theta(s_0)$.

If we write that $|V(B)| = b$, using the relation $[\theta'(s_0) - \kappa_g(x_0)] = 0$, this leads first to :

$$\begin{aligned}
\widetilde{b}_1 &= b[\cos(\theta_0) - \theta'(s_0)\sin(\theta_0)(s - s_0) + \kappa_{n,B}(x_0)t] + \mathcal{O}(|y|^2) \\
\widetilde{b}_2 &= b[\sin(\theta_0) + \sin(\theta_0)\kappa_g(x_0)r + \kappa_g(x_0)\cos(\theta_0)(s - s_0)] + \mathcal{O}(|y|^2) \\
\widetilde{b}_3 &= -b\kappa_{n,B}(x_0)r + \mathcal{O}(|y|^2)
\end{aligned} \tag{10.29}$$

and then to :

$$\begin{aligned}
\widetilde{B}_{23} &= b[\cos\theta_0 - \kappa_g(x_0)\cos\theta_0\, r - \kappa_g(x_0)\sin\theta_0\,(s - s_0) \\
&\quad +(\kappa_{n,B}(x_0) - 2\cos\theta_0\,\kappa^M(x_0))t] \\
&\quad +\mathcal{O}(|y|^2) \\
\widetilde{B}_{31} &= b[\sin\theta_0 + \kappa_g(x_0)\cos\theta_0\,(s - s_0) - 2\sin\theta_0\,\kappa^M(x_0)t] \\
&\quad +\mathcal{O}(|y|^2) \\
\widetilde{B}_{12} &= -b\kappa_{n,B}(x_0)r + \mathcal{O}(|y|^2)
\end{aligned} \tag{10.30}$$

By comparison of the curls on the left and right hand side of (10.1) we get the lemma.

10.2 Towards simplified models

If we neglect in addition the terms of order t^2, we get the potential A^{00} whose components are given by :

$$A_1^{00} = bt[\sin\theta_0 \ + \kappa_g(x_0)\cos\theta_0\,(s-s_0)]\ , \tag{10.31}$$

$$A_2^{00} = -bt[\cos\theta_0 \ - \kappa_g(x_0)\cos\theta_0\, r - \kappa_g \sin\theta_0\,(s-s_0)] - b\frac{\kappa_{n,B}}{2}r^2\ , \tag{10.32}$$

and

$$A_3^{00} = 0\ . \tag{10.33}$$

The corresponding magnetic field is :

$$\begin{array}{ll} B_{23}^{00} & = b\cos\theta_0 - b\cos\theta_0\kappa_g r - b\sin\theta_0\,\kappa_g(s-s_0)\ , \\ B_{31}^{00} & = b\sin\theta_0 - b\cos\theta_0\,\kappa_g(s-s_0)\ , \\ B_{12}^{00} & = -b\kappa_{n,B}r\ . \end{array} \tag{10.34}$$

If we neglect in addition the terms corresponding to $t(s-s_0)$, we get the magnetic potential

$$\begin{array}{ll} A_1^{01} & = bt\sin\theta_0 \\ A_2^{01} & = -bt[\cos\theta_0 \ - \kappa_g(x_0)\cos\theta_0\, r] - b\frac{\kappa_{n,B}}{2}r^2\ , \\ A_3^{01} & = 0\ . \end{array} \tag{10.35}$$

The corresponding magnetic field is :

$$\begin{array}{ll} B_{23}^{01} & = b\cos\theta_0 - b\cos\theta_0\kappa_g r\ , \\ B_{31}^{01} & = b\sin\theta_0\ , \\ B_{12}^{01} & = -b\kappa_{n,B}r\ . \end{array} \tag{10.36}$$

But we should probably first start with the model, where we neglect also the terms in $\mathcal{O}(|rt|)$:

$$\begin{array}{ll} \hat{A}_1 & = b\sin\theta_0\, t\ , \\ \hat{A}_2 & = -b\cos\theta_0\, t - \frac{b}{2}\kappa_{n,B}(s_0)r^2\ , \\ \hat{A}_3 & = 0\ . \end{array} \tag{10.37}$$

Neglecting also the geodesic curvature, this leads to the model :

$$(hD_r - \hat{A}_1)^2 + (hD_s - \hat{A}_2)^2 + h^2D_t^2\ . \tag{10.38}$$

11 Comparison lemmas

Although the problem is easier in the case of upper bounds where we work with explicit quasimodes, we need in the two cases (proof of upper bounds and proof of lower bounds) comparison lemmas permitting to control the error made when considering the simplified models.

11.1 A first comparison lemma

We are interested in the energy $q_A^h(u)$, introduced in (8.27), of some function u in $H^2(\Omega)$ such that

$$\text{supp}(u) \ \subset \ Q(x_0) \ , \tag{11.1}$$

where

$$Q(x_0) = \{x \in \Omega; \ (r(x), s(x)) \in (r_0, s_0) + [-h^\delta, h^\delta]^2, \ t(x) \in [0, \epsilon_2]\} \ , \tag{11.2}$$

for some $\delta \in]0,1[$. From now on, we assume in this section that

$$(r(x_0), s(x_0)) = (0, s_0) \ .$$

Lemma 11.1 .
If (11.1) is satisfied, then

$$\begin{array}{l} (1 - C\, h^{2\delta}) q^h_{\tilde{A}^{(2)}}(u) - C\, \|t^{\frac{1}{2}}(hD_x - A)u\|^2 \\ -C\, [q^h_{\tilde{A}^{(2)}}(u)]^{\frac{1}{2}} \cdot \|(h^{3\delta} + h^{2\delta}t + h^\delta t^2 + t^3)u\| \ - C\, \|(h^{3\delta} + h^{2\delta}t + h^\delta t^2 + t^3)u\|^2 \\ \leq q^h_A(u) \\ \leq (1 + Ch^{2\delta})\, q^h_{\tilde{A}^{(2)}}(u) + C\, \|t^{\frac{1}{2}}(hD_x - A)u\|^2 \\ + C\, [q^h_{\tilde{A}^{(2)}}(u)]^{\frac{1}{2}} \cdot \|(h^{3\delta} + h^{2\delta}t + h^\delta t^2 + t^3)u\| \\ \ +C\, \|(h^{3\delta} + h^{2\delta}t + h^\delta t^2 + t^3)u\|^2 \ , \end{array} \tag{11.3}$$

where :

$$\begin{array}{rl} q^h_{\tilde{A}^{(2)}}(u) & = \int_{Q(x_0)} (1 - r\kappa_g(x_0))[|(hD_t - \tilde{A}_3^{(2)})u|^2 \\ & \quad +((1 + 2r\kappa_g(x_0))|(hD_s - \tilde{A}_2^{(2)})u|^2 + |(hD_r - \tilde{A}_1^{(2)})u|^2]\, drdsdt \ , \end{array} \tag{11.4}$$

$\tilde{A}^{(2)}$ *is the second order polynomial part of the Taylor expansion at* x_0 *of* $\widetilde{A}$ *defined in (8.27) :*

$$\tilde{A}^{(2)}(y) = \sum_{|\beta| \leq 2} \frac{\partial^\beta \widetilde{A}}{\partial y^\beta}(0, s_0, 0) \frac{y^\beta}{\beta!} \ ,$$

with $y = (y_1, y_2, y_3) = (r, s - s_0, t)$.
The function $\kappa_g(x_0)$ *is the geodesic curvature at* x_0 *introduced in (8.11).*

We have actually two types of errors in order to control the comparison of $q_A^h(u)$ and $q^h_{\tilde{A}^{(2)}}(u)$.
The first error is that we replace the initial metric in the coordinates (r, s, t) by the new metric (see Lemma 8.3) :

$$g_0^{new} = dt \otimes dt + dr \otimes dr + (1 - 2r\kappa_g(r_0, s_0))ds \otimes ds \ ,$$

with the corresponding

$$|g^{new}|^{\frac{1}{2}} := (1 - r\kappa_g(r_0, s_0)) \ ,$$

and we consider a similar linearization (with respect to r and t) for g^{ij}.
We then observe that, on the support of u, we have :

$$|g|^{\frac{1}{2}} - |g^{new}|^{\frac{1}{2}} = \mathcal{O}(t) + \mathcal{O}(h^{2\delta}) ,$$

$$g^{ij}_{new} - g^{ij} = \mathcal{O}(t) + \mathcal{O}(h^{2\delta}) .$$

The second error occurs when replacing A by $\tilde{A}^{(2)}$ and this leads to an error in :

$$A - \tilde{A}^{(2)} = \mathcal{O}(|y|^3) = \mathcal{O}((|t| + h^{\delta})^3) .$$

Once these estimates are satisfied, the lemma follows easily using the Cauchy-Schwarz inequality, after having writen :

$$(hD_y - A) = (hD_y - \tilde{A}^{(2)}) + (A - \tilde{A}^{(2)}) .$$

11.2 A second comparison lemma (case $\theta \equiv 0$)

We now perform a gauge transform and a change of unknown in order to go back to the Lebesgue measure. We also decide to consider as remainder the term in $\mathcal{O}(t^2)$ in A. We recall from (8.38) that, in this case

$$\kappa_g(x_0) = 0 ,$$

for $x_0 \in \Gamma$.

Lemma 11.2 .
If (11.1) and (9.2) are satisfied, then

$$\begin{array}{l} q^h_{A^{00}}(v) - C\|t^{\frac{1}{2}}(hD_x - A)u\|^2 \\ -C[q^h_{A^{00}}(v)]^{\frac{1}{2}} \cdot \|(h^{3\delta} + h + h^{2\delta}t + t^2)u\| \\ -C\|(h^{3\delta} + h + h^{2\delta}t + t^2)u\|^2 \\ \leq q^h_A(u) \\ \leq q^h_{A^{00}}(v) + C\|t^{\frac{1}{2}}(hD_x - A)u\|^2 \\ +C[q^h_{A^{00}}(v)]^{\frac{1}{2}} \cdot \|(h^{3\delta} + h + h^{2\delta}t + t^2)u\| \\ +C\|(h^{3\delta} + h + h^{2\delta}t + t^2)u\|^2 \end{array} \tag{11.5}$$

where

$$v = e^{-ip^0/h}u , \tag{11.6}$$

$$q^h_{A^{00}}(v) = \int_{Q(x_0)} [|hD_t v|^2 + |(hD_s - A^{00}_2)v|^2 + |hD_r v|^2]\, drdsdt , \tag{11.7}$$

$$A^{00}_2(r,t;s_0) := -bt - \frac{b}{2}\kappa_{n,B}(x_0)r^2 , \tag{11.8}$$

and where p^0 is the polynomial function introduced in Lemma 10.1.

Lemma 11.2 comes easily from Lemmas 11.1 and 10.1 which give that

$$\begin{array}{l} q^h_{A^{00}}(v) - C[q^h_{A^{00}}(v)]^{\frac{1}{2}} \cdot [h\|u\| + \|t^2u\|] - C[h^2\|u\|^2 + \|t^2u\|^2] \\ \leq q^h_{\widetilde{A}^{(2)}}(u) \\ \leq q^h_{A^{00}}(v) + C[q^h_{A^{00}}(v)]^{\frac{1}{2}} \cdot [h\|u\| + \|t^2u\|] + C[h^2\|u\|^2 + \|t^2u\|^2] . \end{array}$$

12 Spectral theory for a simple model

12.1 Heuristics

We would like to understand the following simplified model considered in (10.38) :

$$P_0 := (hD_r - \sin\theta\, t)^2 + (hD_s + \cos\theta\, t + \gamma\frac{r^2}{2})^2 + h^2 D_t^2 \tag{12.1}$$

on $I\!R^2 \times I\!R^+$. Here θ is assumed to be fixed and γ is a real parameter. We have moreover assumed for simplification assumed that $b = 1$.
We will take later

$$\gamma = \kappa_{n,B}(s_0)\ ,\ \theta = \theta(s_0)\ , \tag{12.2}$$

but it is better to keep them as an independent parameter for the first part of the analysis.

We are interested in the analysis of the bottom of the spectrum but will concentrate on the research of L^2 normalized solutions u^h such that : $\langle P_0 u^h\ ,\ u^h\rangle$ is minimal. .

Scaling .
We first introduce the following scaling : $t = h^{\frac{1}{2}}\tilde{t}$, $r = h^{\frac{1}{3}}\tilde{r}$ and the coefficients of the operator being independent of s we take a Fourier transform in s.

Dividing by h, we get that P_0/h is unitary equivalent to :

$$P_1 := (h^{\frac{1}{6}} D_{\tilde{r}} - \sin\theta\tilde{t})^2 + (h^{\frac{1}{2}}\sigma + \cos\theta\tilde{t} + \gamma h^{\frac{1}{6}}\frac{\tilde{r}^2}{2})^2 + D_{\tilde{t}}^2 \tag{12.3}$$

on $I\!R^2 \times I\!R^+$. We can rewrite the operator in the form :

$$\begin{aligned} P_1 \quad &= D_{\tilde{t}}^2 + \left(\tilde{t} - h^{\frac{1}{6}}\left[\sin\theta D_{\tilde{r}} + \cos\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)\right]\right)^2 \\ &\quad + h^{\frac{1}{6}}\left(\cos\theta D_{\tilde{r}} - \sin\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)\right)^2 . \end{aligned} \tag{12.4}$$

We note that we have "formally " a lower bound of the type :

$$\begin{aligned} P_1 \quad &\geq \mu(h^{\frac{1}{6}}\sin\theta D_{\tilde{r}} + \cos\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)) \\ &\quad + \left(h^{\frac{1}{6}}\cos\theta D_{\tilde{r}} - \sin\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)\right)^2 , \end{aligned} \tag{12.5}$$

which leads naturally to first consider the operator :

$$\begin{aligned} P_2 \quad &:= \mu(h^{\frac{1}{6}}\sin\theta D_{\tilde{r}} + \cos\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)) \\ &\quad + \left(h^{\frac{1}{6}}\cos\theta D_{\tilde{r}} - \sin\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)\right)^2 , \end{aligned} \tag{12.6}$$

now considered as an operator on $L^2(I\!R^2_{\tilde{r},\sigma})$. In order to find a suitable quasi-mode, it is better to first decompose it as an Hilbertian integral of operators

$P_2(\sigma)$, this time defined on $L^2(I\!R)$, and to look for a minimization on σ. In this context, it is natural to replace μ by its approximation at the bottom. We recover a differential model, which will give a good understanding of the problem, modulo an error term which has to be controlled.

We consequently analyze the family (depending on σ)

$$\begin{aligned} P_3(\sigma) \quad &:= \Theta_0 + \delta_0(h^{\frac{1}{6}}(\sin\theta D_{\tilde{r}} + \cos\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)) - \xi_0)^2 \\ &\quad + h^{\frac{1}{3}}\left(\cos\theta D_{\tilde{r}} - \sin\theta(h^{\frac{1}{3}}\sigma + \tfrac{\gamma}{2}\tilde{r}^2)\right)^2 . \end{aligned} \tag{12.7}$$

with $\delta_0 = \frac{1}{2}\mu''(\xi_0)$.

It is now better to introduce,

$$\sigma(\theta) = -\xi_0\cos\theta\ ,\ \rho(\theta) = +\xi_0\sin\theta\ , \tag{12.8}$$

$$\sigma = \sigma(\theta)h^{-\frac{1}{2}} + h^{-\frac{1}{3}}\hat{\sigma}\ , \tag{12.9}$$

which permits to rewrite $P_3(\sigma)$ in the form :

$$\begin{aligned} P_3(\sigma) \quad &:= \Theta_0 + \delta_0(h^{\frac{1}{6}}(\sin\theta(D_{\tilde{r}} + \rho(\theta)h^{-\frac{1}{6}}) + \cos\theta(\hat{\sigma} + \tfrac{\gamma}{2}\tilde{r}^2)))^2 \\ &\quad + h^{\frac{1}{3}}\left(\cos\theta(D_{\tilde{r}} + \rho(\theta)h^{-\frac{1}{6}}) - \sin\theta(\hat{\sigma} + \tfrac{\gamma}{2}\tilde{r}^2)\right)^2 . \end{aligned}$$

A translation in $\hat{\sigma}$ and a gauge transform by $\exp ih^{-\frac{1}{6}}\rho(\theta)r$ leads then to the analysis of the family :

$$\begin{aligned} P_4(\hat{\sigma}) \quad &:= \Theta_0 + h^{\frac{1}{3}}\delta_0((\sin\theta D_{\tilde{r}} + \cos\theta(\hat{\sigma} + \tfrac{\gamma}{2}\tilde{r}^2)))^2 \\ &\quad + h^{\frac{1}{3}}\left(\cos\theta D_{\tilde{r}} - \sin\theta(\hat{\sigma} + \tfrac{\gamma}{2}\tilde{r}^2)\right)^2 . \end{aligned} \tag{12.10}$$

12.2 Analysis of the simplified model

It is then natural to introduce :

$$P_5(\hat{\sigma}) := h^{-\frac{1}{3}}(P_4(\hat{\sigma}) - \Theta_0)\ , \tag{12.11}$$

which becomes independent of h :

$$\begin{aligned} P_5(\hat{\sigma}) \quad &= \delta_0\left(\cos\theta(\tfrac{\gamma}{2}r^2 + \hat{\sigma}) + \sin\theta D_r\right)^2 \\ &\quad + \left(\cos\theta D_r - \sin\theta(\tfrac{\gamma}{2}r^2 + \hat{\sigma})\right)^2 . \end{aligned} \tag{12.12}$$

Here we have omitted the tilde's for the next computations.
Our aim is to minimize over $\hat{\sigma}$ (and then to minimize over the points of Γ, remembering that $\gamma = \kappa_{n,B}(x)$ and $\theta = \theta(x)$ with x on Γ).

Let us now show, that by a gauge transform, we can rewrite $P_5(\hat{\sigma})$ in the form :

$$P_6(\hat{\sigma}) = cD_r^2 + d(r^2 - \rho)^2\ . \tag{12.13}$$

We look for a gauge transformation of the form :

$$t(\theta, r) = \alpha(\theta)(\frac{\gamma}{6} r^3 + \hat{\sigma} r) \, . \tag{12.14}$$

We consider

$$P_6(\hat{\sigma}) := \exp -it(\theta, r) \cdot P_5(\hat{\sigma}) \cdot \exp it(\theta, r) \, . \tag{12.15}$$

The function $\alpha(\theta)$ in (12.14) is chosen such that the coefficients of the operator $(\frac{\gamma}{2} r^2 + \hat{\sigma}) D_r + D_r (\frac{\gamma}{2} r^2 + \hat{\sigma})$ vanishes. This leads to :

$$\alpha(\theta) = \frac{\sin\theta \, \cos\theta \, (1 - \delta_0)}{\delta_0 \sin^2\theta + \cos^2\theta} \, . \tag{12.16}$$

Of course, we have

$$c = \cos^2\theta + \delta_0 \sin^2\theta \, , \tag{12.17}$$

and

$$\rho = 2\hat{\sigma}/\gamma \, . \tag{12.18}$$

But for this value of $\alpha(\theta)$, we get :

$$d = (\frac{\gamma}{2})^2 \left(\delta_0 (\cos\theta + \alpha(\theta) \sin\theta)^2 + (-\sin\theta + \alpha(\theta) \cos\theta)^2 \right) \, .$$

After computation, this gives :

$$d = (\delta_0 (\frac{\gamma}{2})^2) / (\delta_0 \sin^2\theta + \cos^2\theta) \, , \tag{12.19}$$

We now rescale the operator $cD_r^2 + d(r^2 - \rho)^2$. We recall, that we deleted the tilde's for simplicity. But we come back to the former writing[5] and consider :

$$P_6(\hat{\sigma}) = cD_{\tilde{r}}^2 + d(\tilde{r}^2 - \rho)^2 \, .$$

This means that we perform a new scaling :

$$\tilde{r} = (\frac{c}{d})^{\frac{1}{6}} r' \, ,$$

such that $P_6(\hat{\sigma})$ becomes in the new coordinates :

$$P_7(\hat{\sigma}) = d^{\frac{1}{3}} c^{\frac{2}{3}} \left((D_{r'}^2 + ((r')^2 - \rho')^2 \right) \, , \tag{12.20}$$

with

$$\rho' = (\frac{c}{d})^{-\frac{1}{3}} \rho \, .$$

We observe that c and d are independent of $\hat{\sigma}$. So in order to minimize over σ the bottom of the spectrum of the initial operator, we will have to minimize

[5] This is better, if we want to follow all the scalings we have done in the construction of quasimodes.

over ρ', the bottom of the spectrum of $\left(D_{r'}^2 + ((r')^2 - \rho')^2\right)$ which is obtained for $\rho' = \rho_{min}$ and take the value $\hat{\nu}_0$ introduced in (2.14). This corresponds to

$$\hat{\sigma} = \frac{\gamma}{2} \, (\frac{c}{d})^{\frac{1}{3}} \, \rho_{min} \, , \tag{12.21}$$

with

$$\frac{c}{d} = (\cos^2\theta + \delta_0 \sin^2\theta)^2 (\delta_0 (\frac{\gamma}{2})^2)^{-1} \, . \tag{12.22}$$

So, the bottom of the spectrum of P_7, is given for this value of $\hat{\sigma}$ by :

$$d^{\frac{1}{3}} c^{\frac{2}{3}} \hat{\nu}_0 = (\frac{1}{2})^{\frac{2}{3}} \delta_0^{\frac{1}{3}} |\gamma|^{\frac{2}{3}} (\delta_0 \sin^2\theta + \cos^2\theta)^{\frac{1}{3}} \hat{\nu}_0 \, . \tag{12.23}$$

If we now remember the values of γ and θ in our application, this leads to :

Proposition 12.1 .
The ground state energy of the model operator P_4 is given by :

$$\inf_{\hat{\sigma}} \inf \mathrm{Sp} \, P_4(\hat{\sigma}) = \Theta_0 + h^{\frac{1}{3}} \hat{\nu}_0 (\frac{1}{2})^{\frac{2}{3}} \delta_0^{\frac{1}{3}} |\gamma|^{\frac{2}{3}} (\delta_0 \sin^2\theta + \cos^2\theta)^{\frac{1}{3}} \, . \tag{12.24}$$

Moreover the minimum is obtained for $\hat{\sigma}$ defined in (12.21).

In our application γ and θ are not independent but satisfy (12.2) for some x in Γ. This suggests that we have to look for a minimum over Γ of the expression :

$$\gamma^2 \left(\delta_0 \sin^2\theta(x) + \cos^2\theta(x)\right) \, ,$$

that is :

$$\ell^2 := \inf_{x \in \Gamma} \left((\kappa_{n,B}(x))^2 (\delta_0 \sin^2\theta(x) + \cos^2\theta(x)) \right) . \tag{12.25}$$

13 Proof of Theorem 9.2: upper bounds in general

13.1 Analysis of the case when $\theta \equiv 0$

In order to help the reader, we first treat the particular case when $\theta \equiv 0$. Let us show the upper bound in the estimate (9.3) of Theorem 9.1.

Analysis of the model .
Taking into account the assumtion (9.2) and (8.38), the model operator is, (see Lemma 11.2),

$$P^{h,N,0} = h^2 D_r^2 + (hD_s + bt + \frac{b}{2} \kappa_{n,B}(x_0) r^2)^2 + h^2 D_t^2 \tag{13.1}$$

associated to the Neumann problem in the t-variable for $t \in]0, +\infty[$, and the Dirichlet problem for the variables $(r, s) \in I \times J$.
Here I and J are intervals in $I\!R$, which may depend on h. For the moment, we

take $I = J =]-h^\delta, h^\delta[$ and we look for a test function u satisfying (11.1) in the form (cf (11.6))

$$u = e^{ip^0/h}\tilde{u} \ , \tag{13.2}$$

with

$$\tilde{u}(r,s,t) = ch^{-\frac{\delta}{2}} e^{-i\rho\kappa^0_{n,B}\, s/(2h^{\frac{1}{3}})} e^{-ib^{\frac{1}{2}}\xi_0 s/h^{\frac{1}{2}}} \chi(h^{-\delta}C^{-1}s) v(r,t) \tag{13.3}$$

where c is a normalization constant, ρ is a fixed constant which will be defined later on, χ is an even function on $\mathbb{R}$ supported on $[-\frac{1}{2}, \frac{1}{2}]$ and equal to 1 on $[-\frac{1}{4}, \frac{1}{4}]$.
As $s \mapsto \chi^h(s) := ch^{-\frac{\delta}{2}}\chi(h^{-\delta}C^{-1}s)$ is an even function and

$$\|hD_s\chi^h\|^2_{L^2(\mathbb{R}_s)} \leq Ch^{2-2\delta} \ ,$$

we have just to search for a normalized function $v(r,t)$ satisfying

$$q^h_{M^{00}}(v) \leq [hb\Theta_0 + h^{\frac{4}{3}}b^{\frac{2}{3}}\hat{\nu}_0(\mu''(\xi_0))^{\frac{1}{3}}\gamma_0 + C\, h^{\eta+\frac{4}{3}}] \tag{13.4}$$

with

$$q^h_{M^{00}}(v) := \int_{h^\delta Q_2} [|hD_r v|^2 + |M^{00}_2 v|^2 + h^2|D_t v|^2]\, drdt \ , \tag{13.5}$$

$Q_2 =]-C, C[\times[0, C[$, and

$$M^{00}_2(r,t) = b^{\frac{1}{2}}(b^{\frac{1}{2}}t - h^{\frac{1}{2}}\xi_0) + \frac{b}{2}\kappa^0_{n,B}(r^2 - h^{\frac{2}{3}}b^{-1}\rho) \ . \tag{13.6}$$

We introduce the scaling $b^{\frac{1}{2}}(h^{-\frac{1}{3}}r, h^{-\frac{1}{2}}t) = (\hat{r}, \hat{t})$ and take v in the form :

$$v(r,t) = b^{\frac{1}{2}}h^{-\frac{5}{12}}\ v_0(\hat{r}, \hat{t}) \ .$$

We then delete the hats and we get easily that

$$q^h_{M^{00}}(v) = bh\ \tilde{q}^h(v_0) \tag{13.7}$$

with

$$\tilde{q}^h(v_0) := \int_{Q^h} [|D_t v_0|^2 + |[t - \xi_0 + h^{\frac{1}{6}}\frac{b^{-\frac{1}{2}}}{2}\kappa^0_{n,B}(r^2 - \rho)v_0|^2 + h^{\frac{1}{3}}|D_r v_0|^2]\, drdt \ , \tag{13.8}$$

$$Q^h =]-h^{\delta-\frac{1}{3}}b^{\frac{1}{2}}C, h^{\delta-\frac{1}{3}}b^{\frac{1}{2}}C[\times[0, h^{\delta-\frac{1}{2}}b^{\frac{1}{2}}[\ .$$

Let $\varphi_0(t)$ the normalized eigenfunction of $Q(\xi_0)$ associated to the groundstate energy Θ_0 (cf Subsection 2.2). Then one can check easily as in [HeMo2] that

$$\|Q(\xi)\phi^\xi - [\Theta_0 + \frac{1}{2}(\xi - \xi_0)^2\mu''(\xi_0)]\phi^\xi\| \leq C|\xi - \xi_0|^3 \ , \tag{13.9}$$

if $|\xi - \xi_0| \leq c_0$, for some sufficiently small constant c_0, where

$$\phi^\xi(t) = \varphi_0(t) + (\xi - \xi_0)\varphi_1(t) + (\xi - \xi_0)^2\varphi_2(t), \tag{13.10}$$

$$\varphi_1 = 2[Q(\xi_0) - \Theta_0]^{-1,r}[(t-\xi_0)\varphi_0]$$

and

$$\varphi_2 = 2[Q(\xi_0) - \Theta_0]^{-1,r}[(t-\xi_0)\varphi_1 - < (t-\xi_0)\varphi_1 | \varphi_0 > \varphi_0] \, .$$

Here $(Q(\xi_0) - \Theta_0)^{-1,r}$ is the regularized resolvent defined by :

$$\begin{array}{ll} (Q(\xi_0) - \Theta_0)^{-1,r}\varphi_0 & = 0 \, , \\ (Q(\xi_0) - \Theta_0)^{-1,r}u & = (Q(\xi_0) - \Theta_0)^{-1}u \quad \text{if } \langle u|\varphi_0\rangle = 0 \, . \end{array}$$

Let ψ_0 be the normalized eigenfunction (cf Subsection 2.4) associated to the groundstate energy of the Hamiltonian $D_r^2 + (r^2 - \rho_{min})^2$ on $L^2(I\!R)$ and

$$\begin{array}{l} \int_{I\!R}[|D_r\psi_0|^2 + (r^2-\rho_{min})^2|\psi_0|^2]dr \\ = \hat{\nu}_0 \\ = \inf_{\eta \in I\!R} \inf\{\int_{I\!R}[|D_r f|^2 + (r^2-\eta)^2|f|^2]dr; \ \|f\| = 1\} \, . \end{array} \tag{13.11}$$

We recall that $r \mapsto \psi_0(r)$ is an even function.
We take

$$\rho = \alpha^{-2}(b)\rho_{min} \text{ with } \alpha(b) = [\frac{1}{8}\mu''(\xi_0)b^{-1}(\kappa_{n,B}(x_0))^2]^{\frac{1}{6}} \, , . \tag{13.12}$$

$$v_0(r,t) = \psi_0(\alpha(b)r)\phi^{\xi(h,r)}(t)\chi(Ch^{-\delta+\frac{1}{3}}r)\chi(Ch^{-\delta+\frac{1}{2}}t) \, ,$$

with

$$\xi(h,r) = \xi_0 - h^{\frac{1}{6}}\frac{b^{-\frac{1}{2}}}{2}\kappa^0_{n,B}(r^2-\rho) \, .$$

As $r \mapsto v_0(r,t)$ is an even function, we get easily that

$$\tilde{q}^h(v_0) \leq [\Theta_0 + \hat{\nu}_0\alpha^2(b)h^{\frac{1}{3}} + C\,h^{\frac{1}{2}}]\|v_0\|^2 \, .$$

Conclusion of the proof .
The upper bound in (9.3) follows with δ equal to $\frac{5}{16}$ and $\eta = \frac{1}{24}$, in (9.3). Here we take x_0 in Γ such that

$$|\kappa_{n,B}(x_0)| = \inf_{x\in\Gamma}|\kappa_{n,B}(x)| \, . \tag{13.13}$$

13.2 Upper bounds in the generic case

We have seen in the previous subsection how one can heuristically get a candidate for the main term of the ground state. We give now the rigorous proof of the upper bound.

Proposition 13.1 .
Let $P^{h,N}$ be the Neumann magnetic Laplace operator on $L^2(\Omega)$ $(hD-A)^2$, where Ω is a bounded open set of $I\!R^3$ with smooth boundary $\partial\Omega$. We assume that the magnetic field $H = \operatorname{curl} A$ is constant, that

$$\Gamma = \{x \in \partial\Omega; \ H \in T_x(\partial\Omega)\} \text{ is a finite collection of smooth closed curves.} \tag{13.14}$$

and that :

$$\forall\, x \in \Gamma, \quad \kappa^G(x) \neq 0\,. \tag{13.15}$$

Then there exist $\eta > 0$ *and* $C_0 > 0$ *such that, for all* $h \in]0,1]$,

$$\inf \mathrm{Sp}\,(P^{h,N}) \leq hb\Theta_0 + h^{\frac{4}{3}} b^{\frac{2}{3}} \hat{\nu}_0 (\mu''(\xi_0))^{\frac{1}{3}} \gamma_0 + C_0\, h^{\eta+\frac{4}{3}}; \tag{13.16}$$

where $b = |H|$, $\hat{\nu}_0$ *is introduced in (2.14) and*

$$\gamma_0 = \inf_{x\in\Gamma} \tilde{\gamma}(x), \tag{13.17}$$

$$\begin{aligned} \tilde{\gamma}(x)^3 \quad &= \tfrac{1}{8}(\kappa^G(x))^2 \left[\kappa_n^2(x) + \tfrac{1}{2}\mu''(\xi_0) K_x^2(T(x), T(x)\wedge N(x))\right] \times \\ &\quad \times \left[\kappa_n^2(x) + K_x^2(T(x), T(x)\wedge N(x))\right]^{-2}\,. \end{aligned} \tag{13.18}$$

Remark 13.2 .
Let us remark that when the assumptions of Theorem 9.1 are satisfied,

$$K_x(T(x), T(x)\wedge N(x)) = 0 \text{ on } \Gamma\,,$$

so (13.16) is the same upperbound given in (9.3) of the same theorem.

If $\kappa^G \neq 0$, *then* $\kappa_{n,B}$ *is different of* 0. *Note that if we assume in addition that*

$$\kappa_n(x) \neq 0\,,$$

then H *can not be tangent to* Γ. *This would mean indeed that* $\theta = \frac{\pi}{2}$, *and by (8.34) and (8.37) that* $K_{22} = 0$.

Proof of Proposition 13.1 .
Any constant independent of h will be denoted by C. We still use the notation $b = |H|$.
As for the proof of the upper bound in (9.3) of Theorem 9.1, we have just to find an L^2 normalized function u, supported in $h^\delta Q$, with $Q =]-C, C[^2 \times [0, C[$, such that

$$q^h_{A^{00}}(u) := \int_{h^\delta Q} [|(hD_r - A_1^{00})u|^2 + (1+2\kappa_g^0 r)|(hD_s - A_2^{00})u|^2 + h^2|D_t u|^2]\, drdsdt \tag{13.19}$$

satisfies

$$q^h_{A^{00}}(u) \leq \Theta_0 b\, h + b^{\frac{2}{3}} \hat{\nu}_0 (\mu''(\xi_0))^{\frac{1}{3}} \gamma_0\, h^{\frac{4}{3}} + C\, h^{\eta+\frac{4}{3}} \tag{13.20}$$

for some $\delta \in]\frac{5}{18}, \frac{1}{3}[$ and some $\eta > 0$,
and

$$h^{-1}\|(1 + h^{-\frac{1}{4}} t^{\frac{1}{2}})(hD_y - \tilde{A})u\|^2 + \|(1 + h^{-\frac{1}{2}} t)^2 u\|^2 \leq C\,; \tag{13.21}$$

with

$$\begin{aligned} A_1^{00}(r,s,t) \quad &= bt[\sin\theta_0 \;+\; \kappa_g^0 \cos\theta_0\; s]\,, \\ A_2^{00}(r,s,t) \quad &= bt[-\cos\theta_0 \;+\; \kappa_g^0 \cos\theta_0\; r \;+\; \kappa_g^0 \sin\theta_0\; s] - \tfrac{b}{2}\kappa^0_{n,B} r^2\,, \\ \theta_0 \quad &= \theta(x_0) = \arcsin(|<T(x_0)|\tfrac{H}{b}>|)\,, \\ \kappa_g^0 \quad &= \kappa_g(x_0)\,, \\ \kappa^0_{n,B} \quad &= \kappa_{n,B}(x_0)\,, \end{aligned} \tag{13.22}$$

and where $x_0 \in \Gamma$ is chosen such that

$$\tilde{\gamma}(x_0) = \gamma_0 \ .$$

We have chosen a system of coordinates (r, s, t) such that : $x_0 = (0, 0, 0)$. We recall that A^{00} was introduced in (10.31)-(10.33).
We search for a function of the form

$$\begin{aligned} &u(r,s,t;h) = \\ &\quad ch^{-\frac{\delta}{2}} \exp(-\tfrac{i}{h^{\frac{1}{3}}}\rho\kappa^0_{n,B}s) \cdot \exp(\tfrac{i}{h^{\frac{1}{2}}}(\sin\theta_0 r - \cos\theta_0 s)b^{\frac{1}{2}}\xi_0) \cdot \chi(h^{-\delta}C^{-1}s)\ v(r,t) \ , \end{aligned} \tag{13.23}$$

where c is a normalization constant, ρ is a constant to be determined later, χ is an even function on $\mathbb{R}$ supported on $[-\frac{1}{2}, \frac{1}{2}]$ and equal to 1 on $[-\frac{1}{4}, \frac{1}{4}]$.
As $s \mapsto \chi^h(s) := ch^{-\frac{\delta}{2}}\chi(h^{-\delta}C^{-1}s)$ is an even function and

$$\|(hD_s - b\kappa^0_g \sin\theta_0 st)\chi^h\|^2_{L^2(\mathbb{R}_s)} \leq C(h^{2-2\delta} + h^{2\delta}t^2) \ ,$$

we have just to search for a normalized function $v(r,t)$ satisfying

$$q^h_{M^{00}}(v) \leq hb\Theta_0 + h^{\frac{4}{3}}b^{\frac{2}{3}}\hat{\nu}_0(\mu''(\xi_0))^{\frac{1}{3}}\gamma_0 + C\,h^{\eta+\frac{4}{3}} \ , \tag{13.24}$$

with

$$q^h_{M^{00}}(v) := \int_{h^\delta Q_2} [|(hD_r - M^{00}_1)v|^2 + |M^{00}_2 v|^2 + h^2|D_t v|^2]\ drdt \ , \tag{13.25}$$

$Q_2 =]-C, C[\times[0, C[$, and

$$\begin{aligned} M^{00}_1(r,t) &= b^{\frac{1}{2}}\sin\theta_0(b^{\frac{1}{2}}t - h^{\frac{1}{2}}\xi_0) \\ M^{00}_2(r,t) &= (1 + 2\kappa^0_g r)[-b^{\frac{1}{2}}\cos\theta_0(b^{\frac{1}{2}}t - h^{\frac{1}{2}}\xi_0) + \kappa^0_g \cos\theta_0 brt \\ &\qquad -\tfrac{b}{2}\kappa^0_{n,B}(r^2 - h^{\frac{2}{3}}b^{-1}\rho)] \ . \end{aligned} \tag{13.26}$$

Moreover v must satisfy

$$h^{-1}\int_{h^\delta Q_2}(1 + h^{-\frac{1}{2}}t)[|(hD_r - M^{00}_1)v|^2 + |M^{00}_2 v|^2 + h^2|D_t v|^2]\ drdt \leq C \ , \tag{13.27}$$

and

$$\|(1 + h^{-\frac{1}{2}}t)^2 v\|^2 \leq C \ . \tag{13.28}$$

So we can neglect the tr^2 and r^3 terms in M^{00}_2 which will lead to error terms in (13.24), and we get the new

$$\begin{aligned} M^{01}_1(r,t) &:= b^{\frac{1}{2}}\sin\theta_0(b^{\frac{1}{2}}t - h^{\frac{1}{2}}\xi_0) \\ M^{01}_2(r,t) &:= -b^{\frac{1}{2}}\cos\theta_0(b^{\frac{1}{2}}t - h^{\frac{1}{2}}\xi_0) + h^{\frac{1}{2}}b^{\frac{1}{2}}\xi_0\kappa^0_g\cos\theta_0 r - \tfrac{b}{2}\kappa^0_{n,B}(r^2 - h^{\frac{2}{3}}b^{-1}\rho) \ . \end{aligned} \tag{13.29}$$

We introduce the scaling $b^{\frac{1}{2}}(h^{-\frac{1}{3}}r, h^{-\frac{1}{2}}t) = (\hat{r}, \hat{t})$ and take v in the form :

$$v(r,t) = b^{\frac{1}{2}}h^{-\frac{5}{12}}\ v_0(\hat{r}, \hat{t}) \ .$$

We then delete the hats and we get easily that

$$q^h_{M^{01}}(v) = bh\ \tilde{q}^h(v_0) \tag{13.30}$$

with

$$\tilde{q}^h(v_0) := \int_{Q^h} [|D_t v_0|^2 + |(t - \xi_0 - h^{\frac{1}{6}} L^h_1(r, D_r))v_0|^2 + h^{\frac{1}{3}} |L^h_2(r, D_r))v_0|^2]\ drdt\ , \tag{13.31}$$

$$Q^h =]-Cb^{\frac{1}{2}}h^{\delta-\frac{1}{3}}, Cb^{\frac{1}{2}}h^{\delta-\frac{1}{3}}[\times[0, h^{\delta-\frac{1}{2}}b^{\frac{1}{2}}[\ ,$$

and with

$$\begin{aligned} L^h_1(r, D_r) &= \sin\theta_0\, D_r - \cos\theta_0\, \tfrac{b^{-\frac{1}{2}}}{2}[\kappa^0_{n,B}(r^2 - \rho) - 2h^{\frac{1}{6}}\xi_0\kappa^0_g \cos\theta_0\, r]\ ; \\ L^h_2(r, D_r) &= \cos\theta_0\, D_r + \sin\theta_0\, \tfrac{b^{-\frac{1}{2}}}{2}[\kappa^0_{n,B}(r^2 - \rho) - 2h^{\frac{1}{6}}\xi_0\kappa^0_g \cos\theta_0\, r]\ . \end{aligned} \tag{13.32}$$

We search for a function v_0 such that

$$\|(1 + r^2)v_0\| \leq C\|v_0\|.$$

We can neglect terms with $h^{\frac{1}{6}}$ in factor, and the L^h_j are replaced by :

$$\begin{aligned} L^0_1(r, D_r) &= \sin\theta_0\, D_r - \cos\theta_0\, \tfrac{b^{-\frac{1}{2}}}{2}[\kappa^0_{n,B}(r^2 - \rho)]\ ; \\ L^0_2(r, D_r) &= \cos\theta_0\, D_r + \sin\theta_0\, \tfrac{b^{-\frac{1}{2}}}{2}[\kappa^0_{n,B}(r^2 - \rho)]\ . \end{aligned} \tag{13.33}$$

By (13.9) and using Fourier transform, we know that there exist functions $\varphi_j(t),\ j = 0, \ldots, 2$ exponentially decreasing at infinity on $[0, +\infty[$, with their derivatives, such that, for any $\psi \in \mathcal{S}(I\!R)$, if

$$w^h(r, t) = \varphi_0(t)\psi(r) + \varphi_1(t)h^{\frac{1}{6}}L^0_1(r, D_r)\psi(r) + \varphi_2(t)h^{\frac{1}{3}}(L^0_1(r, D_r))^2\psi(r), \tag{13.34}$$

then we get,

$$\begin{aligned} &\|[D_t^2 + (t - \xi_0 - h^{\frac{1}{6}}L^0_1(r, D_r))^2 - (\Theta_0 + \tfrac{1}{2}\mu''(\xi_0)h^{\frac{1}{3}}(L^0_1(r, D_r))^2)]w^h\| \\ &\leq C_e h^{\frac{1}{2}}\|L^0_1(r, D_r))^3\, w^h\|. \end{aligned} \tag{13.35}$$

This is indeed a consequence of the estimate, for $\tau \in I\!R$ and

$$w(t) = \phi_0 + \tau\phi_1 + \tau^2\phi_2\ .$$

$$\|[D_t^2 + (t - \xi_0 - \tau)^2 - (\Theta_0 + \frac{1}{2}\mu''(\xi_0)\tau^2)]w\| \leq C_e|\tau|^3\ , \tag{13.36}$$

and of a suitable functional calculus.

The inequality (13.36) was already used for $|\tau| \leq \tau_0$ in (13.9) but let us just observe that it is also true for $|\tau| > \tau_0 > 0$, if one realizes that the square of the left hand side of (13.36) is a polynomial of degree 4 with respect to the τ variable.

For defining the functional calculus, we can, for example, when $\theta_0 \neq 0$, use a gauge transform which transforms L_1^h into $\sin\theta_0 D_r$ and the proof can then be done by partial Fourier transform. In the case when $\theta_0 = 0$ a direct proof can be done. Note that the constant C_e is independent of θ_0.

Let us define

$$M(r, D_r) := \frac{1}{2}\mu''(\xi_0) L_1^0(r, D_r)^2 + L_2^0(r, D_r)^2 \ . \tag{13.37}$$

At this point, we have justified the heuristic part of the previous section and can use the results obtained on the model. Let

$$\psi^0(r) = (\frac{c}{d})^{-\frac{1}{12}} \ \exp i\varphi(r) \ \psi_0((\frac{c}{d})^{-\frac{1}{6}} r) \tag{13.38}$$

and

$$\psi = \psi^0 \cdot \chi(C^{-1} h^{-\delta+\frac{1}{3}} r) \ . \tag{13.39}$$

We take

$$\rho = b^{\frac{1}{3}} (\frac{c}{d})^{\frac{1}{3}} \rho_{min} \ , \tag{13.40}$$

with c and d as in (12.22), with $\gamma = \kappa^0_{n,B}$ and $\theta = \theta_0$.

We then consider, with $w^h(r,t)$ defined in (13.34) with (13.39),

$$v_0(r,t) = w^h(r,t)\chi(\frac{1}{C}\, h^{-\delta+\frac{1}{2}} t) \ . \tag{13.41}$$

We recall that ψ_0 is exponentially deacreasing at infinity with all its derivatives. Then we get easily from (13.35) and (12.24) that

$$\tilde{q}^h_{A^{00}}(v_0) \leq [\Theta_0 + h^{\frac{1}{3}} \hat{\nu}_0 b^{-\frac{1}{3}} \hat{\gamma}_1 + C\, h^{\frac{1}{2}}] \cdot \|v_0\|^2 \ , \tag{13.42}$$

with

$$\hat{\gamma}_1 = (\frac{1}{2})^{\frac{2}{3}} \delta_0^{\frac{1}{3}} |\kappa^0_{n,B}|^{\frac{2}{3}} (\delta_0 \sin^2\theta_0 + \cos^2\theta_0)^{\frac{1}{3}} \ . \tag{13.43}$$

This gives (13.24) using Remark 9.3.

13.3 Upper bounds in a degenerate case

Proposition 13.3 .
Under the assumptions of Proposition 6.1 and if moreover there exists $x_0 \in \partial\Omega$ such that the Gauss curvature at x_0 vanishes, H is tangent to $\partial\Omega$ at x_0 and the normal curvature at x_0 along the vector H vanishes :

$$H \ \in \ T_{x_0}\partial\Omega \ , \ \kappa^G(x_0) = 0 \ , \ K_{x_0}(H,H) = 0 \ , \tag{13.44}$$

then the upper bound is of the form

$$\lambda(h) \leq b\Theta_0 h + C_0\, h^{\frac{3}{2}} \ . \tag{13.45}$$

Proof of Proposition 13.3.
Let Γ be the geodesic of $\partial\Omega$ through x_0 and normal to H. We consider the coordinates, in a neighbourhood of W_0 of x_0, given by Lemma 8.3, and associated to Γ. Let us remark that the geodesic curvature of Γ vanishes, because Γ is a geodesic.
Then, if $y = (y_1, y_2, y_3) = (r, s, t)$ are the adapted coordinates in a neighbourhood of W_0, and if $\widetilde{b}_j$ are the new components of the vector magnetic field :

$$H = \widetilde{b}_1(y)\frac{\partial}{\partial r} + \widetilde{b}_2(y)\frac{\partial}{\partial s} + \widetilde{b}_3(y)\frac{\partial}{\partial t} ,$$

then, assuming $y(x_0) = 0$,

$$\widetilde{b}_1(0) = b, \;\; \widetilde{b}_2(0) = \widetilde{b}_3(0) = 0 . \tag{13.46}$$

As $\widetilde{b}_j =< H|\frac{\partial}{\partial y_j} >$ and as H is constant, using (8.6), we get

$$\frac{\partial \widetilde{b}_3}{\partial r}(0) =< H|\frac{\partial N}{\partial r}(x_0) >= -bK_{11}(x_0), \; \frac{\partial \widetilde{b}_3}{\partial s}(0) =< H|\frac{\partial N}{\partial s}(x_0) >= -bK_{12}(x_0) . \tag{13.47}$$

But the assumption (13.44) leads to

$$K_{11}(x_0) = K_{12}(x_0) = 0 , \tag{13.48}$$

so (13.47) and (13.48) shows that

$$\begin{array}{l} \widetilde{b}_1 = b + b_{11}r + b_{12}s + b_{13}t + \mathcal{O}(|y|^2) \\ \widetilde{b}_2 = b_{21}r + b_{22}s + b_{23}t + \mathcal{O}(|y|^2) \\ \widetilde{b}_3 = b_{33}t + \mathcal{O}(|y|^2) . \end{array} \tag{13.49}$$

But the asymptotic behavior (8.29) and (8.19) (with $\kappa_g = 0$) prove that

$$|g| = 1 - 4t\kappa^M(x_0) + \mathcal{O}(|y|^2) . \tag{13.50}$$

Then, in the new cordinates, the magnetic potential $\widetilde{A}$ satisfies by (5.11), (5.12) ($H = V(B)$), (13.49) and (13.50)

$$\begin{array}{l} \widetilde{B}_{23} = b + \beta_{11}r + \beta_{12}s + \beta_{13}t + \mathcal{O}(|y|^2) \\ \widetilde{B}_{31} = \beta_{21}r + \beta_{22}s + \beta_{23}t + \mathcal{O}(|y|^2) \\ \widetilde{B}_{12} = \beta_{33}t + \mathcal{O}(|y|^2) . \end{array} \tag{13.51}$$

Then we can choose a gauge $\tilde{A}$ such that

$$\tilde{A}_1(y) = tS_1(y) + \mathcal{O}(|y|^3), \; \tilde{A}_2(y) = -tb + tS_2(y) + \mathcal{O}(|y|^3), \; \tilde{A}_3(y) = 0 , \tag{13.52}$$

where $y \mapsto S_j(y)$ is the linear form

$$S_j(y) = S_{j1}r + S_{j2}s + S_{j3}t .$$

Using again (8.19) with $\kappa_g = 0$ we get that

$$||g|^{\frac{1}{2}}(y)g^\star(X,X) - |X|^2| \leq C\ (t+|y|^2)|X|^2\ ,\ \forall\ X\ \in\ I\!R^3\ . \tag{13.53}$$

As in the proof of (6.1, we get, if $\mathrm{supp}(u)\ \subset\ \{x;\ |x-x_0| \leq h^\delta\}$ with $\delta > 0$, that, for some constant $C = C(\delta) > 0$, independent of h and u,

$$\begin{array}{rl} q_A^h(e^{i\varphi}u) & \leq (1+h^{2\delta}C)q_{A^0}^h(u) \\ & +C\|t^{\frac{1}{2}}(hD_y - \widetilde{A})u\|^2 \\ & +C[h^{3\delta}(q_{A^0}^h(u))^{\frac{1}{2}}\cdot\|u\| + h^{6\delta}\|u\|^2]\ , \end{array} \tag{13.54}$$

where $\varphi(y)$ a real function,

$$A_1^0 = tS_1(y),\ A_2^0 = -bt + tS_2(y),\ A_3^0 = 0\ ,$$

and $q_{A^0}^h(u)$ defined as in (6.7) .
We take the function u of the form

$$u = e^{-ib^{\frac{1}{2}}y_2\xi_0/h^{\frac{1}{2}}}\ v(y)\ ,$$

with v as in (6.8), and we get easily from (13.54) with $\delta = \frac{1}{4}$, that

$$q_A^h(e^{i\varphi}u) \leq (b\Theta_0 h + C\ h^{\frac{3}{2}})\|u\|^2$$

and (13.45) follows.

14 Proof of Theorem 9.1: accurate lower bounds in a particular case.

14.1 Introduction

Before to enter into the technicalities, let us explain the ideas which lead to the partion of unity we shall consider.

We cut $\overline{\Omega}$ in different zones.

- The first zone corresponds to the points which are far from the boundary. They are treated rather easily, exactly as in the case of dimension 2. Here the model with constant magnetic field in $I\!R^3$ is relevant. This corresponds to the introduction of $\Gamma^0_{\tau(h)}$ already done in (7.16). The other zones correspond to a finer decomposition of $\Gamma^1_{\tau(h)}$ also already introduced in (7.16).

- The second zone $\Gamma^{11}\tau(h)$ corresponds to the points which are near Γ at a distance which is $\mathcal{O}(h^\delta)$. The model which was analyzed in the previous sections is essentially relevant.

- The third zone $\Gamma^{13}_{\tau(h)}$ corresponds to the points which are near $\partial\Omega$ but far from Γ. Here the model analyzed in Section 3 is relevant.

- Unfortunately, we need an intermediate zone This will correspond to the introduction of $\Gamma^{12}_{\tau(h)}$ corresponding to points near Γ but not in the second zone. In some sense, we need to be able to interpolate between the second zone and the third zone.

Then, we have to glue together the estimates introduced in each zone and to control the errors related to the partition.

14.2 A partition of unity

We proceed as in the proof of Proposition 7.2 . In the partition of unity (7.14), we take

$$\tau(h) = h^\delta \quad \text{with } \delta \in]\frac{5}{18}, \frac{1}{3}[\, . \tag{14.1}$$

Let us denote by u^h a normalized eigenfunction associated to the ground state energy $\lambda(h)$ of $P^{h,N}$:

$$u^h \in H^1(\Omega), \quad \|u^h\| = 1, \; \lambda(h)\|u^h\|^2 = q^h_A(u^h) \leq q^h_A(v)/\|v\|^2, \; \forall v \in H^1(\Omega) \, . \tag{14.2}$$

As announced in Subsection 14.1, we split $\Gamma^1_{\tau(h)}$, which was defined by (7.16), in the following way. For $C_1 > 1$ fixed large enough, let us define

$$\begin{array}{l} \Gamma^{11}_{\tau(h)} = \{\gamma \in \Gamma^1_{\tau(h)}; \; \text{dist } (\text{supp}(\chi_{\gamma,\tau(h)}), \Gamma) < C_1\tau(h)\} \\ \Gamma^{12}_{\tau(h)} = \{\gamma \in \Gamma^1_{\tau(h)}; \; C_1\tau(h) \leq \text{ dist } (\text{supp}(\chi_{\gamma,\tau(h)}), \Gamma) < C_1^{-1}\} \\ \Gamma^{13}_{\tau(h)} = \{\gamma \in \Gamma^1_{\tau(h)}; \; C_1^{-1} \leq \text{ dist } (\text{supp}(\chi_{\gamma,\tau(h)}), \Gamma)\} \, . \end{array} \tag{14.3}$$

14.3 First zone : $\Gamma^0_{\tau(h)}$

This was already analyzed in Subsection 7.3. We established in (7.18), that :

Lemma 14.1 .

$$\sum_{\gamma \in \Gamma^0_{\tau(h)}} q^h_A(\chi_{\gamma,\tau(h)} u^h) \geq hb \sum_{\gamma \in \Gamma^0_{\tau(h)}} \|\chi_{\gamma,\tau(h)} u\|^2 \, . \tag{14.4}$$

14.4 Second zone : $\Gamma^{11}_{\tau(h)}$

We assume that $\text{supp}(\chi_{\gamma,\tau(h)}) \subset Q(x_0)$ with $x_0 \in \Gamma$ and $Q(x_0)$ satisfying (11.2).
We begin by establishing a lower bound of the ground state energy of the model operator. We consider the model operator (13.1), (coming from Lemma 11.2), on $L^2(I \times J \times \mathbb{R}_+)$ with $I = J = [-C\,h^\delta, C\,h^\delta]$, for some $\delta > 0$ and $C > 0$, and Dirichlet condition on $\partial I \times J \times \mathbb{R}_+ \cup I \times \partial J \times \mathbb{R}_+$ and Neumann condition on $I \times J \times \{0\}$.
We estimate from below its ground state energy by the ground state energy associated to the periodic conditions on a larger interval containing J, for example

on $L^2(I \times \Gamma \times I\!R_+)$. We denote in the same way this operator by $P^{h,N,0}$. Using Parseval formula we get

$$\mathrm{Sp}\,(P^{h,N,0}) = \cup_{k\in\mathbb{Z}} \mathrm{Sp}\,(P_k^{h,N,0}) \tag{14.5}$$

where,

$$P_k^{h,N,0} = h^2 D_t^2 + [\frac{2k\pi}{|\Gamma|}h + tb + \frac{r^2}{2}b\kappa_{n,B}(x_0)]^2 + h^2 D_r^2$$

is defined on $L^2(I \times I\!R_+)$ with the Dirichlet condition on $\partial I \times I\!R_+$ and the Neumann condition on $I \times \{0\}$. For simplicity we assume that the length of the curve Γ is 2π, $|\Gamma| = 2\pi$. So

$$P_k^{h,N,0} = h^2 D_t^2 + [kh + tb + \frac{r^2}{2}b\kappa_{n,B}(x_0)]^2 + h^2 D_r^2 \tag{14.6}$$

Then we have, for the suitable realizations

$$\inf \mathrm{Sp}\,(P_k^{h,N,0}) \geq \inf \mathrm{Sp}\,(h^2 D_r^2 + \mu_k^h(r)), \tag{14.7}$$

where $\mu_k^h(r)$ is the ground state energy of the Neumann problem on $L^2(I\!R_+)$ associated to

$$P_{r,k}^{h,N,0} = h^2 D_t^2 + [kh + tb + \frac{r^2}{2}b\kappa_{n,B}(x_0)]^2 \ .$$

By scaling, we have

$$\mathrm{Sp}\,(P_{r,k}^{h,N,0}) = hb \times \mathrm{Sp}\,(Q(\xi_{h,k}(r))), \tag{14.8}$$

with

$$\xi_{h,k}(r) = -b^{-\frac{1}{2}}h^{-\frac{1}{2}}[kh + \frac{r^2}{2}b\kappa_{n,B}(x_0)], \tag{14.9}$$

and $Q(\xi)$ is defined in (2.4).

Now, as $|r| \leq h^\delta$, with $\delta > 1/4$,

$$|\xi_{h,k}(r) - \xi_0| \leq Ch^{-\tau_0+\frac{1}{6}}$$

when

$$k \ \in \ I_0(h) := [-Ch^{-\tau_0-\frac{1}{3}} - h^{-\frac{1}{2}}\xi_0, -h^{-\frac{1}{2}}\xi_0 + Ch^{-\tau_0-\frac{1}{3}}],$$

and

$$|\xi_{h,k}(r) - \xi_0| \geq \frac{1}{C}h^{-\tau_0+\frac{1}{6}} \ ,$$

when

$$|k - h^{-\frac{1}{2}}\xi_0| \geq C|h^{-\tau_0-\frac{1}{3}}\xi_0| \ .$$

Here τ_0 is non negative, choosen small enough, for example

$$\tau_0 = \min\{\delta - \frac{1}{4}, \ \frac{1}{36}\} \ . \tag{14.10}$$

So we can use (13.9) to get that, for some constant $C_0 > 0$,

$$Q(\xi_{h,k}(r))) \geq \Theta_0 + \frac{1}{C_0} h^{-2\tau_0+\frac{1}{3}}, \text{ if } k \notin I_0(h) , \tag{14.11}$$

so, if $k \notin I_0(h)$, then

$$\inf \mathrm{Sp}\,(h^2 D_r^2 + \mu_k^h(r)) \geq \ hb\Theta_0 + \frac{1}{C_0} h^{-2\tau_0+\frac{4}{3}}, \tag{14.12}$$

Now, we have just to consider the case when $k \in I_0(h)$.
We use also (13.9) to get

$$Q(\xi_{h,k}(r))) \geq \Theta_0 + \frac{\mu''(\xi_0)}{2}(\xi_{h,k}(r) - \xi_0)^2 - Ch^{-3\tau_0+\frac{1}{2}} . \tag{14.13}$$

By using min-max principle, the ground state energy of the Dirichlet problem on I is less then the one on $I\!R$, and then by scaling we get that

$$\begin{array}{l} \inf \mathrm{Sp}\,(h^2 D_r^2 + \mu_k^h(r)) \geq -Ch^{-3\tau_0+\frac{3}{2}} \\ \quad +h \inf \mathrm{Sp}\,\{b\Theta_0 + \frac{1}{2}h^{\frac{1}{3}}(b^2\mu''(\xi_0)\kappa_{n,B}^2(x_0))^{\frac{1}{3}}[D_r^2 + (r^2 - \rho_{h,k})^2]\} , \end{array} \tag{14.14}$$

with

$$-\rho_{h,k} = \sqrt{2}h^{-\frac{1}{6}}(b^2\mu''(\xi_0)\kappa_{n,B}^2(x_0))^{-\frac{1}{6}}[\xi_0 + h^{\frac{1}{2}}\frac{1}{\sqrt{2}}k\kappa_{n,B}^{\frac{1}{2}}(x_0)]),$$

and then, if $k \in I_0(h)$,

$$\begin{array}{l} \inf \mathrm{Sp}\,(h^2 D_r^2 + \mu_k^h(r)) \geq \\ hb\Theta_0 + \frac{1}{2}h^{\frac{4}{3}}\hat{\nu}_0(b^2\mu''(\xi_0)\kappa_{n,B}^2(x_0))^{\frac{1}{3}} - Ch^{-3\tau_0+\frac{3}{2}} . \end{array} \tag{14.15}$$

Then, using a modified version of Lemma 11.1, where $q^h_{\tilde{A}^{(2)}}(u)$ and $q^h_A(u)$ are interchanged, and also Lemma 11.2 (with $q^h_{A^{00}}(u)$ and $q^h_A(u)$ interchanged), we get easily from (14.5), (14.7), (14.10), (14.12) and (14.15), the following lemma

Lemma 14.2 .
Let $\delta \in]\frac{1}{4}, \frac{1}{3}[$, $C_0 > 0$. Then there exists $\tilde{C}_0$ such that, for any $x_0 \in \Gamma$, for any $u \in H^1(\Omega)$ such that

$$\mathrm{supp}(u) \subset \{x \in \overline{\Omega};\ |x - x_0| \leq C_0 h^\delta\} ,$$

for any $h \in]0,1]$, we have :

$$\begin{array}{l} q_A^h(u) \geq [hb\Theta_0 + h^{\frac{4}{3}}\frac{\hat{\nu}_0}{2}[\mu''(\xi_0)\kappa_{n,B}^2(x_0)]^{\frac{1}{3}}]\|u\|^2 \\ -\tilde{C}_0\|t^{\frac{1}{2}}(hD_x - A)u\|^2 - \tilde{C}_0[q_A^h(u)]^{\frac{1}{2}} \cdot \|(h^{3\delta} + h + h^{2\delta}t + t^2)u\| \\ -\tilde{C}_0\|(h^{\delta+\frac{1}{2}} + h^{3\delta} + h + h^{2\delta}t + t^2)u\|^2 \end{array} \tag{14.16}$$

This lemma and (7.1) prove that for the ground state eigenfunction defined in (14.2), we have, for any $\epsilon > 0$,

$$\begin{array}{l} q_A^h(\chi_{\gamma,\tau(h)}u^h) \geq [hb\Theta_0 + h^{\frac{4}{3}}\hat{\gamma}_0 b^{\frac{2}{3}}]\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ -C(h^{1+\epsilon} + h^{6\delta-\epsilon})\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ \qquad -C\|t^{\frac{1}{2}}(hD-A)\chi_{\gamma,\tau(h)}u^h\|^2 \\ \qquad -Ch^{-\epsilon}||t^2\,\|\chi_{\gamma,\tau(h)}u^h\|^2\,. \end{array} \tag{14.17}$$

So, choosing $\epsilon = 3\delta - \frac{1}{2}$, we have proved that there exists $C > O$, such that, for any $\gamma \in \Gamma^{11}_{\tau(h)}$ defined by (14.3), we have

$$\begin{array}{l} q_A^h(\chi_{\gamma,\tau(h)}u^h) \geq [hb\Theta_0 + h^{\frac{4}{3}}\hat{\gamma}_0 b^{\frac{2}{3}} - Ch^{\frac{17}{12}}]\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ -Ch^{3\delta+\frac{1}{2}}\|\chi_{\gamma,\tau(h)}u^h\|^2 - C\|t^{\frac{1}{2}}(hD-A)\chi_{\gamma,\tau(h)}u^h\|^2 - Ch^{\frac{1}{2}-3\delta}||t^2\,\chi_{\gamma,\tau(h)}u^h\|^2\,. \end{array} \tag{14.18}$$

Summing over $\gamma \in \Gamma^{11}_{\tau(h)}$, we will obtain

Lemma 14.3 .
There exists $C > O$, such that, for $\delta \in]\frac{1}{4}, \frac{1}{3}[$, there exists C and h_0 such that, for all $h \in]0, h_0]$,

$$\begin{array}{ll} \sum_{\gamma\in\Gamma^{11}_{\tau(h)}} q_A^h(\chi_{\gamma,\tau(h)}u^h) & \geq [hb\Theta_0 + h^{\frac{4}{3}}\hat{\gamma}_0 b^{\frac{2}{3}}]\sum_{\gamma\in\Gamma^{11}_{\tau(h)}}\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ & \quad -Ch^{3\delta+\frac{1}{2}} - Ch^{\frac{17}{12}}\,. \end{array} \tag{14.19}$$

Proof.
Let

$$r^{11}_\gamma(h) := Ch^{3\delta+\frac{1}{2}}\|\chi_{\gamma,\tau(h)}u^h\|^2 + C\|t^{\frac{1}{2}}(hD-A)\chi_{\gamma,\tau(h)}u^h\|^2 + Ch^{\frac{1}{2}-3\delta}||t^2\,\chi_{\gamma,\tau(h)}u^h\|^2\,.$$

We obtain :

$$\begin{array}{ll} \sum_{\gamma\in\Gamma^{11}_{\tau(h)}} r^{11}_\gamma(h) & \leq Ch^{3\delta+\frac{1}{2}}\sum_{\gamma\in\Gamma^{11}_{\tau(h)}}\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ & \quad + Ch^{\frac{1}{2}-3\delta}\sum_{\gamma\in\Gamma^{11}_{\tau(h)}}||t^2\,\chi_{\gamma,\tau(h)}u^h\|^2 \\ & \quad + C\sum_{\gamma\in\Gamma^{11}_{\tau(h)}}\|t^{\frac{1}{2}}(hD-A)\chi_{\gamma,\tau(h)}u^h\|^2\,. \end{array}$$

We use then Proposition 7.1 for the two first terms of the right hand side. The last term is treated in the following way. As for (7.15), we have also

$$\|t^{\frac{1}{2}}(hD-A)u^h\|^2 = \sum_\gamma[\|t^{\frac{1}{2}}(hD-A)\chi_{\gamma,\tau(h)}u^h\|^2 - h^2\|t^{\frac{1}{2}}\,|\nabla\chi_{\gamma,\tau(h)}|u^h\|^2]\,. \tag{14.20}$$

So

$$\sum_{\gamma\in\Gamma^{11}_{\tau(h)}}\|t^{\frac{1}{2}}(hD-A)\chi_{\gamma,\tau(h)}u^h\|^2 \leq C(h^{\frac{3}{2}} + h^{3-2\delta})\,. \tag{14.21}$$

14.5 Third zone : $\Gamma^{13}_{\tau(h)}$

We use the proof of Proposition 7.2. We observe that we are in the first case considered in the proof of this proposition. Formula (7.28) gives that there exists $c_3 > 0$ and $h_0 > 0$ such that, for any $u \in H^1(\Omega)$ and any $h \in]0, h_0]$,

$$q^h_A(\chi_{\gamma,\tau(h)}u) \geq hb(\Theta_0 + c_3)\|\chi_{\gamma,\tau(h)}u\|^2, \quad \forall \gamma \in \Gamma^{13}_{\tau(h)} \, . \tag{14.22}$$

Taking $u = u^h$ and summing over $\gamma \in \Gamma^{13}_{\tau(h)}$, we get

Lemma 14.4 .
There exists $c_3 > 0$ and $h_0 > 0$ such that for any $h \in]0, h_0]$,

$$\sum_{\gamma \in \Gamma^{13}_{\tau(h)}} q^h_A(\chi_{\gamma,\tau(h)}u^h) \geq hb(\Theta_0 + c_3) \sum_{\gamma \in \Gamma^{13}_{\tau(h)}} \|\chi_{\gamma,\tau(h)}u\|^2 \, . \tag{14.23}$$

14.6 Fourth zone : $\Gamma^{12}_{\tau(h)}$

As for the second zone, we assume that : $\mathrm{supp}(\chi_{\gamma,\tau(h)}) \subset Q(x_0)$, but with $x_0 = (r_0, 0, s_0)$, $r_0 \neq 0$. For simplicity of notation, we take $s_0 = 0$. We have also to consider the case when $J = [-C\,h^\delta, C\,h^\delta]$, with $I = r_0 + [-h^\delta, h^\delta]$, but instead of the third zone, with $|r_0|$ small enough. We will also impose $|r_0| \geq Ch^\delta$, with C large enough in order to have the property that the corresponding $I(h)$ is always sufficiently far from 0.

We will also estimate from below the ground state energy of this Dirichlet problem by the one associated to the periodic problem on a larger interval containing J.

Adapted normal forms .

We will make a Taylor expansion at the point $(r_0, 0, 0)$ instead of $(0, 0, 0)$. It comes easily from (10.22-10.24) that

$$V(B)(x_0) = (b + \beta_{10}r_0^2)\frac{\partial}{\partial r} + \beta_{20}r_0^2\frac{\partial}{\partial s} + \beta_{30}r_0\frac{\partial}{\partial t} \tag{14.24}$$

with

$$|\beta_{10}| + |\beta_{20}| \leq C \ , \ |\beta_{30} + b\kappa_{n,B}(x_{00})| \leq C|r_0| \, , \tag{14.25}$$

and $x_{00} \in \Gamma$, such $s(x_{00}) = s(x_0) := 0$).
Moreover, if we write

$$V(B)(x) = \tilde{b}_1(x)\frac{\partial}{\partial r} + \tilde{b}_2(x)\frac{\partial}{\partial s} + \tilde{b}_3(x)\frac{\partial}{\partial t} \, , \tag{14.26}$$

then it comes also from (10.22-10.24) that

$$\begin{array}{l} |\frac{\partial \tilde{b}_1}{\partial r}(x_0)| + |\frac{\partial \tilde{b}_2}{\partial r}(x_0)| + |\frac{\partial \tilde{b}_3}{\partial r}(x_0) + b\kappa_{n,B}(x_{00})| \leq C|r_0| \\ |\frac{\partial \tilde{b}_1}{\partial s}(x_0)| + |\frac{\partial \tilde{b}_2}{\partial s}(x_0)| + |\frac{\partial \tilde{b}_2}{\partial s}(x_0)| \leq C|r_0| \, . \end{array} \tag{14.27}$$

In the same way, we get from (8.18), (8.19), the assumption (9.2) and (8.38) that

$$|\alpha(x_0) - 1| \leq C|r_0| \ . \tag{14.28}$$

So the magnetic field in the coordinates $y = (r - r_0, s, t)$ satisfies

$$\begin{array}{l} \widetilde{B}_{23}(y) = b + \beta_{10} r_0^2 + \beta_{11} r_0 (r - r_0) + \beta_{12} r_0 s + \beta_{13} t + \mathcal{O}(|y|^2) \\ \widetilde{B}_{31}(y) = \beta_{20} r_0^2 + \beta_{21} r_0 (r - r_0) + \beta_{22} r_0 s + \beta_{23} t + \mathcal{O}(|y|^2) \\ \widetilde{B}_{12}(y) = \beta_{30} r_0 + \beta_{31} (r - r_0) + \beta_{32} r_0 s + \beta_{33} t + \mathcal{O}(|y|^2) \ ; \end{array} \tag{14.29}$$

with

$$\begin{array}{l} |\beta_{11}| + |\beta_{12}| + |\beta_{21}| + |\beta_{22}| + |\beta_{23}| + |\beta_{32}| + |\beta_{33}| \leq C \\ |\beta_{30} + b\kappa_{n,B}(x_{00})| + |\beta_{31} + b\kappa_{n,B}(x_{00})| \leq C|r_0| \ . \end{array} \tag{14.30}$$

Then we can after a change of gauge get $\widetilde{A}(y)$ such that

$$\begin{array}{l} |\widetilde{A}_2 + bt - [\beta_{30} r_0 (r - r_0) + \frac{1}{2} \beta_{31} (r - r_0)^2]| \\ + |\widetilde{A}_1| + |\widetilde{A}_3| \\ \leq C \ [t(r_0^2 + |y|) \ + |r_0| \cdot |y|^2], \end{array} \tag{14.31}$$

Here we observe that a term like $\mathcal{O}(|y|^3)$ is controlled by $Cr_0|y|^2$.

We observe indeed that, with

$$A^{00} = (0, -bt + \beta_{30} r_0 (r - r_0) + \frac{1}{2} \beta_{31} (r - r_0)^2, 0) \ ,$$

we have

$$\operatorname{curl} A^{00} = (b, 0, \beta_{30} r_0 + \beta_{31} (r - r_0)) \ .$$

This leads to :

$$\tilde{B} - \operatorname{curl} A^{00} = (\beta_{10} r_0^2, \beta_{20} r_0^2, 0) + |r_0| \mathcal{O}(y) + \mathcal{O}(|y|^2) \ .$$

If we introduce $\tilde{A}^1 = A^{00} + (\beta_{20} r_0^2 t, -\beta_{10} r_0^2 t, 0)$, we get :

$$\tilde{B} - \operatorname{curl} \tilde{A}^1 = \mathcal{O}(|y|^2) \ .$$

We then define :

$$\widetilde{A}(y) = \tilde{A}^1(y) - \int_0^1 \ \Big[y \wedge (\tilde{B}(sy) - \operatorname{curl} \tilde{A}^1(sy)) \Big] \ s \, ds \ ,$$

which has the right property. We refer to [Tha] (Formula (8.153)) for this standard formula which is called the transversal gauge (or Poincaré gauge).

Comparison .
As for Lemma 11.2, we get from (14.31) the following lemma.

Lemma 14.5 .
If (11.1) is satisfied, then

$$\begin{array}{l} q_A^h(u) - C[\| \, (|r_0| + t^{\frac{1}{2}})(hD_x - A)u\|^2 + h^\delta \|(hD_x - A)u\|^2] \\ -C[q_{A^{00}}^h(v)]^{\frac{1}{2}} \cdot \|(h^{2\delta}|r_0| + h + (h^\delta + r_0^2)t + t^2)u\| \\ -C\|(h^{2\delta}|r_0| + h + (h^\delta + r_0^2)t + t^2)u\|^2 \\ \leq q_{A^{00}}^h(v) \\ \leq q_A^h(u) + C[\|(|r_0| + t^{\frac{1}{2}}) \, (hD_x - A)u\|^2 + + h^\delta \|(hD_x - A)u\|^2] \\ +C[q_A^h(u)]^{\frac{1}{2}} \cdot \|(h^{2\delta}|r_0| + h + (h^\delta + r_0^2)t + t^2)u\| \\ +\|(h^{2\delta}|r_0| + h + (h^\delta + r_0^2)t + t^2)u\|^2 \end{array} \tag{14.32}$$

where

$$v = (\alpha(r,s))^{\frac{1}{2}} e^{-ip^0/h} u \, , \tag{14.33}$$

for some smooth real function p^0,

$$q_{A^{00}}^h(v) = \int_{Q(x_0)} [|hD_t v|^2 + |(hD_s - A_2^{00})v|^2 + |hD_r v|^2] \, drdsdt \, , \tag{14.34}$$

$$A_2^{00}(r,t) := -bt + \beta_{30} r_0 (r - r_0) + \frac{1}{2}\beta_{31}(r - r_0)^2 \, , \tag{14.35}$$

and $r_0 = r(x_0)$.

We recall that the constants β_{30} and β_{31} satisfy (14.30), so by the assumption (9.1), there exists $C_0 > 0$, such that, for $|r_0| \leq \frac{1}{C_0}$,

$$C_0^{-1} \leq |\beta_{30}| \, . \tag{14.36}$$

Lower bound for the model .
By translation, scaling and expanding in Fourier series, we get easily that in (14.34), we have

$$q_{A^{00}}^h(v) \geq hb(\inf_{k \in \mathbb{Z}} \inf \mathrm{Sp}\,(H^{h,k})) \times \|v\|^2, \tag{14.37}$$

where $H^{h,k}$ is the selfadjoint operator on $L^2(I(h) \times \mathbb{R}_+)$ defined by imposing a Dirichlet condition on $\partial I(h) \times \mathbb{R}_+$ and a Neumann condition on $I(h) \times \{0\}$, and by considering the differential operator

$$H^{h,k} w = D_r^2 w + D_t^2 w + (t - \xi_{h,k}(r))^2 w, \ \forall v \in C_0^\infty(I(h) \times \mathbb{R}_+) \, . \tag{14.38}$$

Here $I(h) =]-h^{\delta - \frac{1}{2}} b^{\frac{1}{2}}, h^{\delta - \frac{1}{2}} b^{\frac{1}{2}}[$ and

$$\xi_{h,k}(r) = a_0 h^{\frac{1}{2}} r^2 + 2d_0 r - h^{\frac{1}{2}} b^{-\frac{1}{2}} k \, ; \tag{14.39}$$

with $a_0 := -\frac{1}{2}b^{-3/2}\beta_{31}$ and $d_0 := -\frac{1}{2}b^{-1}\beta_{30}r_0$.
So , by (14.30)

$$C^{-1} \leq |a_0| \leq C, \quad \text{and } C^{-1}|r_0| \leq |d_0| \leq C|r_0| \ . \tag{14.40}$$

Then we get that, for the Dirichlet realizations in $I(h)$

$$\inf \mathrm{Sp}\,(H^{h,k}) \geq \inf \mathrm{Sp}\,\left(D_r^2 + \mu(\xi_{h,k}(r))\right) \ . \tag{14.41}$$

Lemma 14.6 .
Let $\delta \in]0, \frac{1}{3}[$. There exist some constants $C_0 \geq 1$ and $c_1 > 0$ such that, for all $(h,k) \in]0,1[\times\mathbb{Z}$, and r_0 s.t.

$$|r_0| \in [C_0 h^\delta, \frac{1}{C_0}] \ , \tag{14.42}$$

we have, for the realization in $I(h)$:

$$\inf \mathrm{Sp}\,(D_r^2 + \mu(\xi_{h,k}(r))) \ \geq \ \Theta_0 + c_1|r_0| \, . \tag{14.43}$$

This lemma comes easily, after a translation in the r variable, from the following one.

Lemma 14.7 .
There exist strictly positive constants c_0 and c_1 such that, for any $\zeta \in \mathbb{R}$, for any $\gamma \neq 0$, the Dirichlet realization of the operator :

$$P_{\zeta,h} := hD_r^2 + \mu(\zeta + \frac{\gamma r^2}{h^{\frac{1}{2}}}) - \Theta_0 \ ,$$

in an open interval $I(h)$ such that :

$$I(h) \subset]0, +\infty[\cup]-\infty, 0[\ ,$$

we have :

$$\langle P_{\zeta,h}u|u\rangle \geq c_0(\inf_{r\in I(h)} \min(|\gamma r|, c_1) \ )||u||^2 \ , \ \forall u \in C_0^\infty(I(h)) \ .$$

Proof.
The proof is based on a bracket argument. According to the properties of μ described in Subsection 2.2, we can find a regular increasing function f such that :

$$\mu(t) - \Theta_0 = (f(t - \xi_0))^2 \ ,$$

with :

$$f(0) = 0 \ , \ f'(t) > 0 \ , \ \lim_{t\to-\infty} f(t) = -\infty \ , \ \lim_{t\to\infty} f(t) = 1 \ .$$

Using the identity :

$$[h^{\frac{1}{2}}D_r \ , \ f(\frac{r^2}{h^{\frac{1}{2}}} + \zeta - \xi_0)] = \frac{2}{i}\gamma r f'(\frac{r^2}{h^{\frac{1}{2}}} + \zeta - \xi_0) \ ,$$

we observe[6] that, according to the assumption that $I(h)$ avoids 0

$$\langle P_{\zeta,h}u|u\rangle \geq 2\langle |r||\gamma|f'(\frac{r^2}{h^{\frac{1}{2}}}+\zeta-\xi_0)u\ ,\ u\rangle\ .$$

and we add the trivial estimate :

$$\langle P_{\zeta,h}u|u\rangle \geq \langle f^2(\frac{r^2}{h^{\frac{1}{2}}}+\zeta-\xi_0)u\ ,\ u\rangle\ .$$

This leads to

$$\begin{array}{ll}\langle P_{\zeta,h}u|u\rangle & \geq \frac{1}{2}\inf_{r\in I(h)}\left(2|r||\gamma|f'(\frac{r^2}{h^{\frac{1}{2}}}+\zeta-\xi_0)+f^2(\frac{r^2}{h^{\frac{1}{2}}}+\zeta-\xi_0)\right)||u||^2\\ & \geq \inf_{r\in I(h)}(|\gamma r|,\frac{1}{2})\inf_{s\in I\!R}(f'(s)+f(s)^2)||u||^2\ .\end{array}$$

We can take $c_1=\frac{1}{2}$ and the lemma will consequently follow from :

$$\inf_{s\in I\!R}(f'(s)+f(s)^2)>0\ .$$

But the proof is easy.

Using Lemma 14.5 and (14.43), we get the following lemma

Lemma 14.8 .
Let $\delta\in\,]0,\frac{1}{3}[$, $C_0>0$. Then there exists $c_0>0$, such that, for any $C_1>0$, there exists $C>0$, such that, for any $x_0\in\partial\Omega$ such that

$$\rho_0:=d(x_0,\Gamma)\in[C_1h^\delta,\frac{1}{C_1}]\ , \tag{14.44}$$

for any u in $H^1(\Omega)$ supported in $\{x\in\overline{\Omega};\ |x-x_0|\leq C_0\,h^\delta\}$, for any $h\in]0,1]$, we have

$$\begin{array}{l}q_A^h(u)\geq[hb\Theta_0+hc_0\rho_0]\|u\|^2\\ -C[\|(\rho_0+t^{\frac{1}{2}})(hD_x-A)u\|^2+h^\delta\|(hD_x-A)u\|^2]\\ -C[q_A^h(u)]^{\frac{1}{2}}\cdot\|(h^{2\delta}\rho_0+h+(h^\delta+\rho_0^2)t+t^2)u\|\\ -C\|h^{2\delta}\rho_0+h+(h^\delta+\rho_0^2)t+t^2)u\|^2\end{array} \tag{14.45}$$

We first deduce :

$$\begin{array}{ll}(1+C\rho_0^2+Ch^\delta)q_A^h(u) & \geq[hb\Theta_0+hc_0\rho_0]\|u\|^2\\ & \quad -C\|t^{\frac{1}{2}})(hD_x-A)u\|^2\\ & \quad -C[q_A^h(u)]^{\frac{1}{2}}\cdot\|(h^{2\delta}\rho_0+h+(h^\delta+\rho_0^2)t+t^2)u\|\\ & \quad -C\|h^{2\delta}\rho_0+h+(h^\delta+\rho_0^2)t+t^2)u\|^2\end{array} \tag{14.46}$$

[6] This is the estimate :

$$||L_1u||^2+||L_2u||^2\geq\pm i\langle[L_1\,,L_2]u\ ,\ u\rangle\ .$$

The mixed term $[q_A^h(u)]^{\frac{1}{2}} \cdot \|(h^{2\delta}\rho_0 + h + (h^\delta + \rho_0^2)t + t^2)u\|$ is to analyze carefully and we analyze each of the terms appearing in its expression.

Let us first consider the term :

$$T_1 = [q_A^h(u)]^{\frac{1}{2}} \cdot \|(h^{2\delta}\rho_0 u\| \ .$$

We use the estimate :

$$T_1 \leq D^{-1}\rho_0 q_A^h(u) + D\rho_0^{-1}\|h^{2\delta}\rho_0 u||^2 \ ,$$

with the idea that we will have to choose D large enough. We have indeed

$$D\rho_0^{-1}\|h^{2\delta}\rho_0 u||^2 = \rho_0 h h^{4\delta-1} D||u||^2 \ .$$

This is OK, for h small enough, under the condition : $\delta > \frac{1}{4}$. We can for example take $D = h^{\frac{1}{2}-2\delta}$.
Let us now consider the second term :

$$T_2 = h^\delta \ [q_A^h(u)]^{\frac{1}{2}} \cdot \|tu\| \ .$$

Here we write :

$$T_2 \leq D^{-1}\rho_0 q_A^h(u) + D\rho_0^{-1}h^{2\delta}||tu||^2 \ ,$$

where D has to be large, and we observe that :

$$D\rho_0|\rho_0^{-1}h^\delta|^2||tu||^2 \leq CD\rho_0 C_1^{-2}||tu||^2 \ .$$

This is essentially OK, if C_1 is large enough because the term $||tu||^2$ is hoped to be of order $\mathcal{O}(h)$. But we have to be careful with this point, which will be treated later.

The third term to consider is :

$$T_3 = [q_A^h(u)]^{\frac{1}{2}} \cdot ||\rho_0^2 tu\| \ .$$

We can use :

$$T_3 \leq D^{-1}\rho_0 q_A^h(u) + (D\rho_0^2)\rho_0||tu||^2 \ ,$$

with again D large.

The other terms are smaller or controlled in the same way. . We can for example use that $\mathcal{O}(t^2)$ is controlled by $\rho_0\mathcal{O}(|t|)$ on the support of u.

This implies the following lemma:

Lemma 14.9 .
There exists $\hat{c}_0 > 0$, C and C_1^0, such that, if C_1 in (14.3) satisfies $C_1 \geq C_1^0$ then, for any $u \in H^1(\Omega)$,

$$\begin{aligned} q_A^h(\chi_{\gamma,\tau(h)}u) \quad &\geq h(b\Theta_0 + \rho_0\hat{c}_0)\,\|\chi_{\gamma,\tau(h)}u\|^2 \\ &\quad -C\,\|t^{\frac{1}{2}}(hD_x - A)\chi_{\gamma,\tau(h)}u\|^2 \\ &\quad -\tfrac{C}{C_1}\rho_0\,||t\chi_{\gamma,\tau(h)}u\|^2 \ , \end{aligned} \tag{14.47}$$

for all $\gamma \in \Gamma^{12}_{\tau(h)}$.

We plan to use this estimate with $u = u^h$ and to sum over the γ's in $\Gamma^{12}_{\tau(h)}$.

Here we meet a problem with the term $\rho_0 \sum_\gamma ||t\chi_\gamma u^h||^2$. Proposition 7.1 can indeed gives that :

$$\frac{C}{C_1}\rho_0 \sum_\gamma ||t\chi_\gamma u^h||^2 \leq \frac{C}{C_1}\rho_0 ||tu^h||^2 \leq \frac{C'}{C_1}\rho_0 h \ ,$$

but this error is much too large and the fact that we can increase C_1 is not enough. One could think that one could get instead the better :

$$\frac{C}{C_1}\rho_0 \sum_{\gamma\in\Gamma^{12}_{\tau(h)}} ||t\chi_\gamma u^h||^2 \leq \frac{C'}{C_1}\rho_0 h \sum_{\gamma\in\Gamma^{12}_{\tau(h)}} ||\chi_\gamma u^h||^2 \ ,$$

but this is probably not true. We will actually show the weaker :

$$\frac{C}{C_1}\rho_0 \sum_{\gamma\in\Gamma^{12}_{\tau(h)}} ||t\chi_\gamma u^h||^2 \leq \frac{C'}{C_1}\rho_0 h \sum_{\gamma\in\Gamma^{12}_{\tau(h)}} ||\chi_\gamma u^h||^2 + \mathcal{O}(h^{2-2\delta}) \ . \tag{14.48}$$

In order to get this more accurate upper bound, we need to get a :

Local control of $||t\chi u^h||$.
We follow the proof of Proposition 7.1, but we have to take account of the presence of χ. One first obtains (see (7.4)) that :

$$\begin{aligned} hb\int t^2\chi^2|u^h|^2 \quad &\leq \int t^2|(hD-A)\chi u^h|^2 \\ &\quad +Ch\|(hD-A)\chi u^h\|\cdot\|t\chi u^h\| \ . \end{aligned}$$

Commuting χ and $(hD-A)$ in the second term of the right hand side, we get :

$$\begin{aligned} hb\int t^2\chi^2|u^h|^2 \quad &\leq \int t^2|(hD-A)\chi u^h|^2 \\ &\quad +Ch\|\chi(hD-A)u^h\|\cdot\|t\chi u^h\| \\ &\quad +Ch\|t\,|\nabla\chi|\,(hD-A)u^h\|\cdot\|t\chi u^h\| \ . \end{aligned} \tag{14.49}$$

Let us now analyze $\int t^2|(hD-A)\chi u^h|^2$. Starting from :

$$\int t^2|(hD-A)\chi u^h|^2 = \int t^2\left(\chi(hD-A)u^h + h\nabla\chi u^h\right)\cdot\left(\overline{\chi(hD-A)u^h + h\nabla\chi u^h}\right) \ ,$$

we get :

$$\begin{aligned} \int t^2|(hD-A)\chi u^h|^2 \quad &\leq \int t^2\chi^2(hD-A)^2u^h\overline{u^h} \\ &\quad +h^2\int t^2|\nabla\chi|^2|u^h|^2 \\ &\quad +2h||t\chi u^h||\,||t(\nabla\chi)\cdot(hD-A)u^h|| \\ &\quad +Ch||t\chi u^h||\,||\chi(hD-A)u^h|| \end{aligned}$$

This leads to

$$\begin{aligned} \int t^2|(hD-A)\chi u^h|^2 \quad &\leq \lambda(h)\int t^2|\chi u^h|^2 \\ &\quad +h^2\int t^2|\nabla\chi|^2|u^h|^2 \\ &\quad +2h||t\chi u^h||\,||t(\nabla\chi)\cdot(hD-A)u^h|| \\ &\quad +Ch||t\chi u^h||\,||t\chi(hD-A)u^h|| \end{aligned}$$

We then get :

$$\begin{aligned}(hb-\lambda(h))\int t^2|\chi u^h|^2 \quad &\leq h^2\int t^2|\nabla\chi|^2|u^h|^2 \\ &\quad +Ch||t\chi u^h||\,||t\chi(hD-A)u^h|| \\ &\quad +Ch\|t\,|\nabla\chi|\,(hD-A)u^h\|\cdot\|t\chi u^h\|\,.\end{aligned}$$

This leads to the estimate :

$$\|t\chi u^h\|^2 \leq C[\,\|\chi(hD-A)u^h\|+\|t|\nabla\chi|(hD-A)u^h\|\,]\;\|t\chi u^h\|+h\int t^2|\nabla\chi|^2|u^h|^2\,.$$

and consequently to

$$\|t\chi u^h\|^2 \leq C[\,\|\chi(hD-A)u^h\|^2+\|t|\nabla\chi|(hD-A)u^h\|^2+h\int t^2|\nabla\chi|^2|u^h|^2\,]\,. \tag{14.50}$$

On the other hand, we have :

$$\|\chi(hD-A)u^h\|^2 \leq \lambda(h)\|\chi u^h\|^2+2\|\chi(hD-A)u^h\|\cdot\|\,|\nabla\chi|\,u^h\|$$

and consequently to :

$$\|\chi(hD-A)u^h\|^2 \leq C\left[h\|\chi u^h\|^2+h^2\|\,|\nabla\chi|\,u^h\|^2\right]\;. \tag{14.51}$$

Finally the two estimates (14.50) et (14.51) give

$$\|t\chi u^h\|^2 \leq C\left[h\|\chi u^h\|^2+h^2\|\,|\nabla\chi|\,u^h\|^2+h\|t\,|\nabla\chi|\,u^h\|^2+\|t\,|\nabla\chi|\,(hD-A)u^h\|^2\right]\;. \tag{14.52}$$

We now take $\chi=\chi_\gamma$ and sum over $\gamma\in\Gamma^{12}_{\tau(h)}$. Using Proposition 7.1, we get, with

$$r^1_\gamma := h^2\|\,|\nabla\chi_\gamma|\,u^h\|^2+h\|t\,|\nabla\chi_\gamma|\,u^h\|^2+\|t\,|\nabla\chi_\gamma|\,(hD-A)u^h\|^2 \tag{14.53}$$

$$\sum_{\gamma\in\Gamma^{12}_{\tau(h)}} r^1_\gamma \leq Ch^{2-2\delta}\,. \tag{14.54}$$

We can treat the second error term in (14.47) as in the second step.

This implies the following lemma:

Lemma 14.10 .
There exists $\tilde{c}_0>0$, C and C^0_1, such that, if C_1 in (14.3) satisfies $C_1\geq C^0_1$ then

$$\begin{aligned}q^h_A(\chi_{\gamma,\tau(h)}u) \quad &\geq h\,(b\Theta_0+\rho_0\tilde{c}_0)\,\|\chi_{\gamma,\tau(h)}u^h\|^2 \\ &\quad -r^{12}_\gamma(h)\,,\end{aligned} \tag{14.55}$$

for all $\gamma\in\Gamma^{12}_{\tau(h)}$, with

$$\sum_{\gamma\in\Gamma^{12}_{\tau(h)}} r^{12}_\gamma \leq C(h^{2-2\delta}+h^{\frac{3}{2}})\,.$$

Because δ will be chosen in $]\frac{1}{4},\frac{1}{3}[$. The last remainder is smaller.

14.7 End of the proof

Then (14.1), (14.23), (14.4 and (7.15) prove that, for $\delta \in]\frac{5}{18}, \frac{1}{3}[$, there exists C and h_0 such that, for all $h \in]0, h_0]$,

$$\lambda(h) \geq [hb\Theta_0 + h^{\frac{4}{3}}\hat{\gamma}_0 b^{\frac{2}{3}}] - C(h^{2-2\delta} + h^{3\delta+\frac{1}{2}}) - Ch^{\frac{17}{12}} \ . \tag{14.56}$$

Then, the lower bound in Theorem 9.1 is obtained by taking for example $\delta = \frac{3}{10}$. This leads to :

$$\lambda(h) \geq [hb\Theta_0 + h^{\frac{4}{3}}\hat{\gamma}_0 b^{\frac{2}{3}}] - Ch^{\frac{7}{5}} \ . \tag{14.57}$$

15 Conclusion

In this article, we have established a conjecture extending Bernoff-Sternberg conjecture in the case of dimension 3. We have proved the upper bound part in full generality and established the lower bound part in a special case. What remains is consequently to prove the lower bound in the conjecture in the general case. As in [HeMo2], we need also to describe the applications to the localization of the ground states which was mentioned in the introduction as our main motivation. We hope to come back to these points in a near future [HeMo4].

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