On the semi-classical analysis of the groundstate energy of the Dirichlet Pauli operator (after Helffer-Persson Sundqvist).

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Abstract

Motivated by a recent paper by Ekholm–Kowarik–Portmann, we analyze the semi-classical analysis of the ground state energy of the Dirichlet-Pauli operator. Tunneling effect can be measured with some analogy with the semi-classical analysis of the small eigenvalues of a Witten Laplacian, as analyzed in papers by Helffer-Sjöstrand, Helffer-Klein-Nier, Helffer-Nier,.... The presented works are in collaboration with Mikael Persson Sundqvist (University of Lund) (two papers [HPS1] and [HPS2]).

Pauli operator

Let Ω be a connected, regular domain in \mathbb{R}^2 , B=B(x) be a magnetic field in $C^\infty(\bar{\Omega})$, and h>0 a semiclassical parameter. We are interested in the analysis of the ground state energy $\lambda_{P_-}^D(h,\mathbf{A},B,\Omega)$ of the Dirichlet realization of the Pauli operator

$$P_{\pm}(h, \mathbf{A}, B, \Omega) := (hD_{x_1} - A_1)^2 + (hD_{x_2} - A_2)^2 \pm hB(x).$$

Here $D_{x_j} = -i\partial_{x_j}$ for j = 1, 2.

The vector potential $\mathbf{A} = (A_1, A_2)$ satisfies

$$B(x) = \partial_{x_1} A_2(x) - \partial_{x_2} A_1(x). \tag{1}$$

The reference to A is not necessary when Ω is simply connected (gauge invariance) but could play a role in the non simply connected case.



The Pauli operator is non-negative on $C_0^{\infty}(\Omega)$. This follows by an integration by parts or think also of the square of the Dirac operator

$$D_A := \sum_j \sigma_j (h D_{x_j} - \mathbf{A}_j),$$

where the σ_j (j=1,2) are the 2×2 -Pauli matrices. We have, on $C_0^{\infty}(\Omega; \mathbb{C}^2)$

$$D_A^2 := (P_-(h, \mathbf{A}, B, \Omega), P_+(h, \mathbf{A}, B, \Omega)).$$

This implies that

$$\lambda_{P_{+}}^{D}(h, \mathbf{A}, B, \Omega) \geq 0.$$

When $\Omega = \mathbb{R}^2$ and B > 0 constant, we have

$$\lambda_{P_-}(h,\mathbf{A},B,\mathbb{R}^2)=0$$
.

When $\Omega = \mathbb{R}^2$ under weak assumptions on B(x) (see Helffer-Nourrigat-Wang (1989), Thaller (book 1992))

$$0 \in \sigma_{ess}(P_{-}(h, \mathbf{A}, B, \mathbb{R}^2)) \cup \sigma_{ess}(P_{+}(h, \mathbf{A}, B, \mathbb{R}^2))$$
.

Is 0 in the kernel ? Aharonov-Casher's theorem (see Cycon-Froese-Kirsch-Simon (book 1986)). What is going on when Ω is bounded ?

Two years ago, T. Ekholm, H. Kowarik and F. Portmann [2] give a lower bound which has a universal character

Theorem EKP

Let Ω be regular, bounded, simply connected in \mathbb{R}^2 . If B does not vanish identically in Ω , $\exists \ \epsilon > 0$ s.t. $\forall h > 0$, $\forall \mathbf{A}$ s.t. $\operatorname{curl} \mathbf{A} = B$,

$$\lambda_{P_{-}}^{D}(h, \mathbf{A}, B, \Omega) \ge \lambda^{D}(\Omega) h^{2} \exp(-\epsilon/h).$$
 (2)

where $\lambda^D(\Omega)$ denotes the ground state energy of the Laplacian on Ω .

Our goal is to determine (when B>0) the optimal ϵ , to give exponentially small upper bounds [8] and to analyze the non simply connected case [9]. This will be done in the semi-classical limit: $h\to 0$.

The main theorem in [8] is

Theorem HPS1

If B(x) > 0, Ω is simply connected and if ψ_0 is the solution of

$$\Delta \psi_0 = B(x) \text{ in } \Omega, \, \psi_{0/\partial\Omega} = 0,$$

then, for any h > 0,

$$\lambda_{P_{-}}^{D}(h, B, \Omega) \ge \lambda^{D}(\Omega) h^{2} \exp(2\inf \psi_{0}/h).$$
 (3)

and, in the semi-classical limit

$$\lim_{h\to 0} h \log \lambda_{P_-}^D(h, B, \Omega) \le 2 \inf \psi_0.$$

In the non simply connected case, such formulation could be wrong. The result could depend on the circulations of the magnetic potential along the different components of the boundary. Below we show that in the semi-classical limit the circulation effects disappear in the rate of the exponential decay.

Theorem HPS2

If B(x) > 0, Ω is connected, and if ψ_0 is the solution of

$$\Delta \psi_0 = B(x) \text{ in } \Omega, \, \psi_{0/\partial\Omega} = 0,$$

then, for any **A** such that $\operatorname{curl} \mathbf{A} = \mathbf{B}$,

$$\lim_{h \to 0} h \log \lambda_{P_{-}}^{D}(h, \mathbf{A}, B, \Omega) = 2 \inf \psi_{0}. \tag{4}$$

We observe that the lower bound in this generalization is no more universal and only true in the semi-classical limit. The proof will use strongly the gauge invariance of the problem.

Canonical choice of the magnetic potential

Following what is done for example in superconductivity, given some magnetic potential $\bf A$ in Ω satisfying curl $\bf A=B$, we can after a gauge transformation assume that $\bf A$ satisfies in addition

$$\operatorname{div} \mathbf{A} = 0 \text{ in } \Omega; \mathbf{A} \cdot \nu = 0 \text{ on } \partial \Omega.$$
 (5)

If this is not satisfied for say A_0 , we can construct

$$\mathbf{A} = \mathbf{A}_0 + \nabla \phi$$

satisfying in addition (5), by choosing ϕ as a solution of

$$-\Delta\phi=\operatorname{div}\mathbf{A}_0$$
 in Ω ; $\nabla\phi\cdot\nu=-\mathbf{A}_0\cdot\nu$ on $\partial\Omega$.

The role of the circulations in the case with holes

The second point to observe is a standard proposition (also present in Hodge-De Rham theory)

Proposition

Let Ω be an open connected set with k holes Ω_j . Given B in $C^{\infty}(\bar{\Omega})$ and k real numbers Φ_j , then there exists a unique $\mathbf{A}(\Phi)$ satisfying (1), (5) and

$$\int_{\partial\Omega_j} \mathbf{A}(\Phi) = \Phi_j \tag{6}$$

Hence, the only relevant parameters in the analysis of spectral problems for the Pauli operator are the magnetic field B and the circulations Φ_i along the boundaries of the holes (if any).

Generating function

Associated with $\mathbf{A} := \mathbf{A}(\Phi)$ satisfying (5), \exists a unique ψ^{Φ} s.t.

$$\mathbf{A}(\Phi) = \nabla^{\perp}\psi^{\Phi}$$

and $\psi^{\Phi}_{/\partial\widetilde{\Omega}}=0$, where $\widetilde{\Omega}$ is the simply connected envelope of Ω .

This ψ^{Φ} is constant on each connected component of the boundary $\partial\Omega$.

If we denote by $p_k(\Phi)$ the value of the trace of ψ^{Φ} on ∂D_k , one can show

Lemma

The map $\mathbb{R}^k \ni \Phi \mapsto p(\Phi) \in \mathbb{R}^k$ is a bijection from \mathbb{R}^k onto \mathbb{R}^k .

We note that Ψ^{Φ} is the unique solution of

$$\Delta \Psi^{\Phi} = B \,,\, \psi^{\Phi}_{/\partial D_k} = p(\Phi) \,,\, \psi^{\Phi}_{/\partial \widetilde{\Omega}} = 0 \,. \tag{7}$$

Remarks and notation

This is a rather standard fact in Hodge-De Rham theory in the case with boundary.

We write

$$\psi_{p} = \psi^{\Phi}$$
, when $p = p(\Phi)$,

where

$$\Delta \Psi_{p} = B, (\psi_{p})_{/\partial D_{k}} = p, (\psi_{p})/\partial \widetilde{\Omega} = 0.$$
 (8)

In the case, with no hole (k = 0), there is no Φ and we recover ψ_0 as given previously.

Variation of the oscillation of $\psi_{ m p}$

The oscillation is defined by

$$\operatorname{Osc}(\psi_p) = \sup \psi_p - \inf \psi_p.$$

When p = 0 and B > 0

$$Osc(\psi_0) = -\inf \psi_0. \tag{9}$$

Using that $p \mapsto \psi_p - \psi_0$ is a linear map, more precisely:

$$\psi_{p} - \psi_{0} = \sum_{j} p_{j} \theta_{j},$$

with

$$0 \le \theta_j \le 1$$
, $(\theta_j)_{\partial D_i} = \delta_{ij}$, $(\theta_j)_{\partial \Omega} = 0$, and $\Delta \theta_j = 0$

we get:

$$|\operatorname{Osc}(\psi_p) - \operatorname{Osc}(\psi_0)| \le \sum_{i} |p_j|.$$
 (10)

Variation of the oscillation of ψ^{Φ}

Similarly, observing that

$$(\Phi - \Phi^0)_j = \sum_{\ell=1}^k M_{j\ell} \, p_\ell$$

with M invertible and Φ^0 the family of circulations such that $p(\Phi^0) = 0$, we get, for some constant C > 0

$$|\operatorname{Osc}(\psi^{\Phi}) - \operatorname{Osc}(\psi_0)| \le C |\Phi - \Phi^0|.$$
 (11)

Isospectrality

In the non simply connected case, it is important to have in mind the following standard proposition:

Proposition

Let $\Omega \subset \mathbb{R}^2$ be bounded and connected, $\mathbf{A} \in C^1(\overline{\Omega})$, $\widetilde{\mathbf{A}} \in C^1(\overline{\Omega})$ satisfying

$$\operatorname{curl} \mathbf{A} = \operatorname{curl} \widetilde{\mathbf{A}} , \qquad (12)$$

and

$$\frac{1}{2\pi h} \int_{\gamma} (\mathbf{A} - \widetilde{\mathbf{A}}) \in \mathbb{Z}, \text{ on any closed path } \gamma \text{ in } \Omega$$
 (13)

then the associated Dirichlet realizations of $(hD - \mathbf{A})^2 + V$ and $(hD - \widetilde{\mathbf{A}})^2 + V$ are unitary equivalent.

This can be applied to the Pauli operator with $V = \pm hB$.

Towards lower bounds: EKP-approach.

To get lower bounds, we consider $\|(hD - \mathbf{A})u\|^2$ by writing

$$u = \exp\left(-\frac{\psi^{\Phi}}{h}\right) v.$$

We have the following identity if A satisfies (1) and (5):

$$||(hD - \mathbf{A})u||^{2} - h \int_{\Omega} B(x)|u(x)|^{2} dx = h^{2} \int_{\Omega} \exp\left(-2\frac{\psi^{\Phi}}{h}\right) |(\partial_{x_{1}} + i\partial_{x_{2}})v|^{2} dx .$$
 (14)

With u (and consequently v) in $H_0^1(\Omega)$, this implies

$$\begin{split} &\|(hD-\mathbf{A})u\|^2 - h\int_{\Omega}B(x)|u(x)|^2\,dx\\ &\geq h^2\exp\Bigl(\frac{-2(\sup\psi^\Phi)}{h}\Bigr)\int_{\Omega}|(\partial_{x_1}+i\partial_{x_2})v|^2\,dx\\ &\geq h^2\exp\Bigl(\frac{-2(\sup\psi^\Phi)}{h}\Bigr)\int_{\Omega}|\nabla v|^2\,dx\\ &\geq h^2\exp\Bigl(\frac{-2\mathrm{Osc}(\psi^\Phi)}{h}\Bigr)\lambda^D(\Omega)\int_{\Omega}|u|^2dx \ . \end{split}$$

So we have obtained

Theorem

Assume that Ω is a bounded connected domain. Then

$$\lambda_{P_{-}}^{D}(h, \mathbf{A}, B, \Omega) \ge h^2 \lambda^{D}(\Omega) \exp\left(\frac{-2\operatorname{Osc}(\psi^{\Phi})}{h}\right).$$
 (15)

Note that the statement is just the statement given in [EKP]-paper, but with a special choice of ψ^{Φ} . This gives the existence of $\epsilon>0$ but we can be far from optimality. When Ω has no hole, we recover when B>0, having in mind (10), the lower bound statement in "Theorem-HPS1" as established in [HPS1].

Implementing gauge invariance

Implementing the gauge invariance and the control of the oscillation established in (11), we obtain

Theorem

Assume that Ω is a bounded connected domain. Then there exists C>0 such that, for any $\Phi\in\mathbb{Z}^k$, any h>0

$$\lambda_{P_{-}}^{D}(h, \mathbf{A}, B, \Omega) \ge h^{2} \lambda^{D}(\Omega) \exp{-\frac{C}{h}} d(\Phi_{0}, \Phi + 2\pi \mathbb{Z}^{k} h) \exp{\left(\frac{-2\operatorname{Osc}(\psi_{0})}{h}\right)}.$$
(16)

When B > 0, we get

$$\lambda_{P_{-}}^{D}(h, \mathbf{A}, B, \Omega) \\ \geq h^{2} \lambda^{D}(\Omega) \exp{-\frac{C}{h}} d(\Phi_{0}, \Phi + 2\pi \mathbb{Z}^{k} h) \exp{\left(\frac{2(\inf{\psi_{0}})}{h}\right)}.$$
 (17)

Upper bounds in the non-simply connected case

In the simply connected case, with the explicit choice of ψ_0 , it is easy to get:

Proposition HPS1

Under assumption B>0 and assuming that Ω is simply connected, we have, for any $\eta>0$, there exists $C_{\eta}>0$

$$\lambda_{P_{-}}^{D}(h,B,\Omega) \le C \exp \frac{2\inf \psi_0}{h} \exp \frac{2\eta}{h}. \tag{18}$$

The proof is obtained by taking as trial state $u=\exp{-\frac{\psi_0}{\hbar}v_\eta}$, with v_η with compact support in Ω and $v_\eta=1$ outside a sufficiently small neighborhood of the boundary and implementing this quasimode in (14). One concludes by the max-min principle.

It has been shown in [HPS1] how to have a (probably) optimal upper bound by using as trial state

$$u = \exp(-\frac{\psi_0}{h}) - \exp(\frac{\psi_0}{h}).$$

This is at least the case for the disk.

In the non simply connected case the situation is much more complicate.

We can get general results by considering an $\tilde{\Omega}$ simply connected in Ω . This proves that $\lambda_{P_-}^D(h, \mathbf{A}, B, \Omega)$ is indeed exponentially small, independently of the circulations along each component of the boundary.

When, for some ψ , ψ_{min} is attained at a point in Ω i.e. if

$$p_j := \psi/\partial\Omega_j > \psi_{\min}, \qquad (19)$$

for $j = 0, \dots, k$, where $\partial \Omega_0 = \partial \tilde{\Omega}$.

In this case, one gets

Proposition

If $\psi/\partial\Omega_j>\psi_{min}$, then, for any $\eta>0$, there exists $C_\eta>0$ and h_η such that, for $h\in(0,h_\eta)$,

$$\lambda_{P_{-}}^{D}(h, \mathbf{A}, B, \Omega) \leq C \exp \frac{2(\inf \psi - \inf_{j} \psi / \partial \Omega_{j})}{h} \exp \frac{2\eta}{h}.$$
 (20)

We observe that the assumption $\psi/\partial\Omega_j>\inf\psi$ is stable when a small variation of the Φ is performed. This assumption is evidently satisfied for B>0 and $\Phi=\Phi_0$.

By gauge transformation, we can find $\alpha \in \mathbb{Z}^k$ such that $\Phi_h := \Phi + 2\pi\alpha h$ is O(h)-close to Φ_0 and similarly $p(\Phi_h)$ is O(h). We can then apply the previous proposition to ψ^{Φ_h} which is close to ψ_0 .

Remark 1

The case $B(x) \leq 0$ can be analyzed further under additional conditions (for example, one could think to start with the case when B(x) has a non degenerate negative minimum at a point of Ω). We refer to Helffer–Mohamed (1996), Helffer–Morame (2002), Helffer–Kordyukov (2014) and Raymond–Vu Ngoc (2016) for the analysis of the Schrödinger with magnetic field, and note that the addition of the term -hB(x) in P_- can be controlled in their analysis.

Remark 2

When B(x) = 2, the solution ψ_0 appears to be $-f_{\tau}$, where f_{τ} is the so-called torsion function which plays an important role in Mechanics.

If Ω is convex, Kawohl has shown that ψ_0 has a unique minimum in Ω .

There are a lot of treated examples in the engineering literature and a lot of mathematical studies, starting from the fifties with Pólya–Szegö. This permits in particular to improve the applications given in [EKP] (see [HPS1]).

Remark 3

The case of the disk is analyzed in detail in [HPS1] in continuation of the works of Erdös, Helffer-Morame, Fournais-Helffer and [EKP].

Theorem HPS1

Assume that $\Omega = D(0, R)$ is the disk of radius R, and that the magnetic field B(x) is constant, B(x) = B > 0.

Then, as $h \to 0^+$,

$$\lambda_{P_{-},0}^{D}(h) = B^{2}R^{2}e^{-BR^{2}/2h}(1 + \mathcal{O}(h)). \tag{21}$$

The case of the annulus is considered in [HPS2].

A Faber-Krahn type Erdős inequality

We also mention a deep result by L. Erdős which is useful in this context.

Proposition

For any planar domain Ω and B>0, let $\lambda^D(h,B,\Omega)$ be the ground state energy of the Dirichlet realization of the semi-classical magnetic Laplacian with constant magnetic field equal to B in Ω . Then we have:

$$\lambda^{D}(h, B, \Omega) \ge \lambda^{D}(h, B, D(0, R)), \qquad (22)$$

where D(0,R) is the disk with same area as Ω :

$$\pi R^2 = \text{Area}(\Omega)$$
.

Moreover the equality in (22) occurs if and only if $\Omega = D(0, R)$.



Dirichlet forms and Witten Laplacians

The problem we study is quite close to the question of analyzing the smallest eigenvalue of the Dirichlet realization of the operator associated with the quadratic form:

$$C_0^{\infty}(\Omega) \ni v \mapsto h^2 \int_{\Omega} |\nabla v(x)|^2 e^{-2f(x)/h} dx$$
. (23)

For this case, we can mention Theorem 7.4 in Freidlin-Wentcell, which says (in particular) that, if f has a unique non-degenerate local minimum x_{min} , then the lowest eigenvalue $\lambda_1(h)$ of the Dirichlet realization $\Delta_{f,h}^{(0)}$ in Ω satisfies:

$$\lim_{h \to 0} -h \log \lambda_1(h) = 2 \inf_{x \in \partial \Omega} (f(x) - f(x_{min})). \tag{24}$$

More precise or general results (prefactors) are given in Bovier-Eckhoff-Gayrard-Klein. This is connected with the semi-classical analysis of Witten Laplacians (Witten, Helffer-Sjöstrand, Cycon-Froese-Kirsch-Simon, Simon, Helffer-Klein-Nier, Helffer-Nier, Lepeutrec, Michel,)

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