Uniform Lieb-Thirring Inequality for the Three-Dimensional Pauli Operator with a Strong Non-Homogeneous Magnetic Field

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Abstract. The Pauli operator describes the energy of a nonrelativistic quantum particle with spin $\frac{1}{2}$ in a magnetic field and an external potential. A new Lieb-Thirring type inequality on the sum of the negative eigenvalues is presented. The main feature compared to earlier results is that in the large field regime the present estimate grows with the optimal (first) power of the strength of the magnetic field. As a byproduct of the method, we also obtain an optimal upper bound on the pointwise density of zero energy eigenfunctions of the Dirac operator. The main technical tools are:

(i) a new localization scheme for the square of the resolvent of a general class of second order elliptic operators;

(ii) a geometric construction of a Dirac operator with a constant magnetic field that approximates the original Dirac operator in a tubular neighborhood of a fixed field line. The errors may depend on the regularity of the magnetic field but they are uniform in the field strength.

1 Introduction
1.1 Notations

Let $B \in C^4(\mathbb{R}^3;\mathbb{R}^3)$ be a magnetic field, $\text{div} \, B = 0$, and $V \in L^1_{\text{loc}}(\mathbb{R}^3)$ a real-valued potential function. Let $A : \mathbb{R}^3 \to \mathbb{R}^3$ be a vector potential generating the magnetic field, i.e., $B = \nabla \times A$. The three-dimensional Pauli operator is the following operator acting on the space of $L^2(\mathbb{R}^3;\mathbb{C}^2)$ of spinor-valued functions:

$$H = H(h, A, V) := \left[ \sigma \cdot (-ih\nabla + A) \right]^2 + V = (-ih\nabla + A)^2 + V(x) + h\sigma \cdot B(x),$$

(1.1)

where $\sigma = (\sigma^1, \sigma^2, \sigma^3)$ is the vector of the Pauli spin matrices, i.e.,

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

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The spectral properties of $H$ depend only on $B$ and $V$ and do not depend on the specific choice of $A$. We shall be concerned only with gauge invariant quantities therefore we can always make the Poincaré gauge choice. In particular, we can always assume that $A$ is at least as regular as $B$ and $V$ and do not depend on the specific choice of $A$. We shall be concerned only with gauge invariant quantities therefore we can always make the Poincaré gauge choice. In particular, we can always assume that $A$ is at least as regular as $B$. The operator $H = H(h, A, V)$ is defined as the Friedrichs’ extension of the corresponding quadratic form from $C_0^\infty(\mathbb{R}^3; \mathbb{C}^2)$.

The Pauli operator describes the motion of a non-relativistic electron, where the electron spin is important because of its interaction with the magnetic field. For simplicity we have not included any physical parameters (i.e., the electron mass, the electron charge, the speed of light, or Planck’s constant $\hbar$) in the expressions for the operators. In place of Planck’s constant we have the semiclassical parameter $\hbar$ and in most of the paper we also set $\hbar = 1$.

The last identity in (1.1) can easily be checked. If we define the three-dimensional Dirac operator

$$D := \sigma \cdot (-i\hbar \nabla + A(x)), \quad (1.2)$$

then we recognize the last identity in (1.1) as the Lichnerowicz’ formula.

The eigenvalues of $H$ below the essential spectrum are of special interest. They determine the possible bound states of a non-relativistic electron subject to the magnetic field $B$ and the external potential $V$. Under very general conditions on $V$ and $B$ one can show that the bottom of the essential spectrum for the Pauli operator is at zero (see [HNW]). This is in sharp contrast to the case of the spinless magnetic Schrödinger operator, $(-i\hbar \nabla + A)^2 + V(x)$, whose essential spectrum is not known in general even for decaying potentials.

Therefore we shall restrict our attention to the negative eigenvalues, $e_1(H) \leq e_2(H) \leq \cdots \leq 0$ of $H$. It is known that under very general conditions there are infinitely many negative eigenvalues even for constant magnetic field [Sol], [Sob-86], however their sum is typically finite. We recall that the sum of the eigenvalues below the essential spectrum is equal to the ground state energy of the noninteracting fermionic gas subject to $H$.

The sum of the negative eigenvalues, $\sum_j e_j(H)$, has been extensively studied recently. In order to find the asymptotic behavior of the ground state energy of a large atom with interacting electrons, one needs, among other things, a semiclassical asymptotics for $\sum_j e_j(H)$ as $h \to 0$.

The semiclassical formula for the sum of the negative eigenvalues is given as

$$E_{sc}(h, B, V) := -\hbar^{-3} \int_{\mathbb{R}^3} P(h|B(x)|, |V(x)|) \, dx \quad (1.3)$$

with

$$P(B, W) := \frac{B}{3\pi^2} \left( W^{3/2} + 2 \sum_{\nu=1}^\infty [2\nu B - W]^{3/2} \right) = \frac{2}{3\pi} \sum_{\nu=0}^\infty d_\nu B [2\nu B - W]^{3/2} \quad (1.4)$$