

Agmon's type estimates of exponential behavior  
of solutions of systems of elliptic partial  
differential equations.

Applications to Schrödinger, Moisi-Theodorescu  
and Dirac operators.

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**Abstract**

The aim of this paper is to derive Agmon's type exponential estimates for solutions of elliptic systems of partial differential equations on  $\mathbb{R}^n$ . We show that these estimates are related with the essential spectra of a family of associated differential operators which depend on the original operator, and with exponential weights which describe the decrease of solutions at infinity. The essential spectra of the involved operators are described by means of their limit operators.

The obtained results are applied to study the problem of exponential decay of eigenfunctions of matrix Schrödinger, Moisi-Theodorescu, and Dirac operators.

## 1 Introduction

The main aim of the paper is to obtain Agmon's type exponential estimates for the decaying behavior of solutions of systems of elliptic partial differential equations with variable coefficients. Exponential decay estimates of this type are intensively studied in the literature. We only mention Agmon's pioneering papers [1, 2] where estimates of eigenfunctions of second order elliptic operators

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were obtained in terms of a special metric, now called the Agmon metric. Exponential estimates for solutions of pseudodifferential equations on  $\mathbb{R}^n$  are also considered in [13, 14, 16, 17, 18, 20, 21, 22].

In this paper, we propose a new approach to exponential estimates for solutions of systems of partial differential equations. Our approach is based on the limit operators method. This method was employed earlier to study the essential spectrum of perturbed pseudodifferential operators, which has found applications to electro-magnetic Schrödinger operators, square-root Klein-Gordon, and Dirac operators under very general assumptions for the magnetic and electric potentials at infinity. Based on the limit operators method, a simple and transparent proof of the well known Hunziker, van Winter, Zhislin theorem (HWZ-Theorem) for multi-particle Hamiltonians was derived in [22, 23]. In [25], the limit operators method was applied to study the essential spectrum of discrete Schrödinger operators.

Let

$$A(x, D)u(x) = \sum_{|\alpha| \leq m} a_\alpha(x) D^\alpha u(x), \quad x \in \mathbb{R}^n$$

be a uniformly elliptic system of partial differential operators of order  $m$  on  $\mathbb{R}^n$  with bounded and uniformly continuous  $N \times N$  matrix-valued coefficients  $a_\alpha$ . Further let  $w := \exp v$  be a weight on  $\mathbb{R}^n$  such that  $\lim_{x \rightarrow \infty} w(x) = \infty$  and assume that all first and higher order derivatives of  $v$  exist and are bounded.

With the operator  $A(x, D)$  and the weight  $w$ , we associate a family of partial differential operators,

$$B_t := A(x, D + it\nabla v(x)), \quad t \in [-1, 1].$$

We let  $\text{sp}_{ess} B_t$  denote the essential spectrum of  $B_t$  considered as an unbounded closed operator on the Hilbert space  $L^2(\mathbb{R}^n, \mathbb{C}^N)$  with domain  $H^m(\mathbb{R}^n, \mathbb{C}^N)$ . Further we let  $L^2(\mathbb{R}^n, \mathbb{C}^N, w)$  and  $H^m(\mathbb{R}^n, \mathbb{C}^N, w)$  refer to the corresponding weighted spaces of vector-valued functions  $u$  such that  $wu \in L^2(\mathbb{R}^n, \mathbb{C}^N)$  and  $wu \in H^m(\mathbb{R}^n, \mathbb{C}^N)$ , respectively. The following result, which will be proved in this paper, provides exponential estimates for the decay of the solutions of the equation  $A(x, D)u = f$ .

**Theorem 1** *Let  $A(x, D)$  be a uniformly elliptic on  $\mathbb{R}^n$  matrix partial differential operator with bounded and uniformly continuous coefficients, and assume that  $0 \notin \text{sp}_{ess} B_t$  for every  $t \in [-1, 1]$ . Let  $u \in H^m(\mathbb{R}^n, \mathbb{C}^N, w^{-1})$  be a solution of the equation  $A(x, D)u = f$  with  $f \in L^2(\mathbb{R}^n, \mathbb{C}^N, w)$ . Then  $u \in H^m(\mathbb{R}^n, \mathbb{C}^N, w)$ .*

By this result, the derivation of exponential estimates of solutions of the equation  $A(x, D)u = f$  is basically reduced to the calculation of the essential spectrum of the  $B_t$ . The latter can be done by means of the limit operators method (see [26, 27] and the monograph [28]). For, one associates with each operator  $B_t$  the family  $\text{op}(B_t)$  of its limit operators  $B_t^g$  which, roughly speaking, describe the behaviour of the operator at infinity. Then it follows from [26, 27, 28] that

$$\text{sp}_{ess} B_t = \bigcup_{B_t^g \in \text{op}(B_t)} \text{sp} B_t^g, \quad (1)$$

where  $\text{sp } B_t^g$  denotes the spectrum of the unbounded operator  $B_t^g$  acting on  $L^2(\mathbb{R}^n, \mathbb{C}^N)$ .

In many important instances, the limit operators are of an enough simple structure, namely partial differential operators with constant coefficients. Then formula (1) provides an effective tool to calculate the essential spectra of partial differential operators and thus, in view of Theorem 1, to get exponential estimates for the solutions of the equation  $A(x, D)u = f$ . We will illustrate this statement by applying Theorem 1 to verify the exponential decay and to obtain explicit exponential estimates for the eigenvectors of Schrödinger operators with matrix potentials, of Moisil-Theodorescu quaternionic operators with variable coefficients, and of Dirac operators.

The contents of the paper is as follows. In Section 2 we introduce the main definitions and prove Theorem 1. The following sections are devoted to several applications of Theorem 1. We start in Section 3 with the essential spectrum and exponential estimates for eigenvectors of Schrödinger operators with matrix potentials. Note that the well known Pauli operator is a Schrödinger operator of this kind (see, for instance, [4]). Moreover, such operators appear in the Born-Oppenheimer approximation for polyatomic molecules [10, 15, 19]. For potentials which are slowly oscillating at infinity we describe the location of the essential spectrum and give exact estimates of the behavior of eigenfunctions of the discrete spectrum at infinity.

In Section 4 we consider general Moisil-Theodorescu (quaternionic) operators with variable coefficients. Note that numerous important systems of partial differential operators of quantum mechanics, elasticity theory, and field theory admit a formulation in terms of quaternionic operators (see [5, 9, 11, 12, 29] and the references cited there). We shall verify explicit necessary and sufficient conditions for quaternionic operators with variable coefficients to be Fredholm operators and derive exponential estimates at infinity for solutions of Fredholm quaternionic equations.

In the concluding Section 5 we consider the Dirac operator on  $\mathbb{R}^3$ , equipped with a Riemannian metric, with electric and magnetic potentials which are slowly oscillating at infinity.

## 2 Exponential estimates of solutions of systems of partial differential equations

### 2.1 Essential spectrum

We will use the following standard notations.

- Given Banach spaces  $X, Y$ ,  $\mathcal{L}(X, Y)$  is the space of all bounded linear operators from  $X$  into  $Y$ . We abbreviate  $\mathcal{L}(X, X)$  to  $\mathcal{L}(X)$ .
- $L^2(\mathbb{R}^n, \mathbb{C}^N)$  is the Hilbert space of all measurable functions on  $\mathbb{R}^n$  with

values in  $\mathbb{C}^N$ , provided with the norm

$$\|u\|_{L^2(\mathbb{R}^n, \mathbb{C}^N)} := \left( \int_{\mathbb{R}^n} \|u(x)\|_{\mathbb{C}^N}^2 dx \right)^{1/2}.$$

- The unitary operator  $V_h$  of shift by  $h \in \mathbb{R}^n$  acts on  $L^2(\mathbb{R}^n, \mathbb{C}^N)$  via  $(V_h u)(x) := u(x - h)$ .
- $C_b(\mathbb{R}^n)$  is the  $C^*$ -algebra of all bounded continuous functions on  $\mathbb{R}^n$ .
- $C_b^u(\mathbb{R}^n)$  is the  $C^*$ -subalgebra of  $C_b(\mathbb{R}^n)$  of all uniformly continuous functions.
- $SO(\mathbb{R}^n)$  is the  $C^*$ -subalgebra of  $C_b^u(\mathbb{R}^n)$  which consists of all functions  $a$  which are slowly oscillating in the sense that

$$\lim_{x \rightarrow \infty} \sup_{y \in K} |a(x + y) - a(x)| = 0$$

for every compact subset  $K$  of  $\mathbb{R}^n$ .

- $SO^1(\mathbb{R}^n)$  is the set of all bounded differentiable functions  $a$  on  $\mathbb{R}^n$  such that

$$\lim_{x \rightarrow \infty} \frac{\partial a(x)}{\partial x_j} = 0 \text{ for } j = 1, \dots, n.$$

Evidently,  $SO^1(\mathbb{R}^n) \subset SO(\mathbb{R}^n)$ .

We also use the standard multi-index notation. Thus,  $\alpha = (\alpha_1, \dots, \alpha_n)$  with  $\alpha_j \in \mathbb{N} \cup \{0\}$  is a multi-index,  $|\alpha| = \alpha_1 + \dots + \alpha_n$  is its length, and

$$\partial^\alpha := \partial_{x_1}^{\alpha_1} \dots \partial_{x_n}^{\alpha_n} \quad \text{and} \quad D^\alpha := (-i\partial_{x_1})^{\alpha_1} \dots (-i\partial_{x_n})^{\alpha_n}$$

are the operators of  $\alpha^{th}$  derivative. Finally,  $\langle \xi \rangle := (1 + |\xi|^2)^{1/2}$  for  $\xi \in \mathbb{R}^n$ .

We consider matrix partial differential operators of order  $m$  of the form

$$(Au)(x) = \sum_{|\alpha| \leq m} a_\alpha(x) (D^\alpha u)(x), \quad x \in \mathbb{R}^n \quad (2)$$

under the assumption that the coefficients  $a_\alpha$  belong to the space

$$C_b^u(\mathbb{R}^n, \mathcal{L}(\mathbb{C}^N)) := C_b^u(\mathbb{R}^n) \otimes \mathcal{L}(\mathbb{C}^N).$$

The operator  $A$  in (2) is considered as a bounded linear operator from the Sobolev space  $H^m(\mathbb{R}^n, \mathbb{C}^N)$  to  $L^2(\mathbb{R}^n, \mathbb{C}^N)$ . The operator  $A$  is said to be *uniformly elliptic* on  $\mathbb{R}^n$  if

$$\inf_{x \in \mathbb{R}^n, \omega \in S^{n-1}} \left| \det \sum_{|\alpha|=m} a_\alpha(x) \omega^\alpha \right| > 0 \quad (3)$$

where  $S^{n-1}$  refers to the unit sphere in  $\mathbb{R}^n$ .

The Fredholm properties of the operator  $A$  can be expressed in terms of its limit operators which are defined as follows. Let  $h : \mathbb{N} \rightarrow \mathbb{R}^n$  be a sequence which tends to infinity. The Arzelà-Ascoli theorem combined with a Cantor diagonal argument implies that there exists a subsequence  $g$  of  $h$  such that the sequences of the functions  $x \mapsto a_\alpha(x + g(k))$  converges as  $k \rightarrow \infty$  to a limit function  $a_\alpha^g$  uniformly on every compact set  $K \subset \mathbb{R}^n$  for every multi-index  $\alpha$ . The operator

$$A^g := \sum_{|\alpha| \leq m} a_\alpha^g D^\alpha$$

is called the *limit operator of  $A$  defined by the sequence  $g$* . Equivalently,  $A^g$  is the limit operator of  $A$  with respect to  $g$  if and only if, for every function  $\chi \in C_0^\infty(\mathbb{R}^n)$ ,

$$\lim_{m \rightarrow \infty} V_{-g(m)} A V_{g(m)} \chi I = A^g \chi I$$

in the space  $\mathcal{L}(H^m(\mathbb{R}^n, \mathbb{C}^N), L^2(\mathbb{R}^n, \mathbb{C}^N))$  and

$$\lim_{m \rightarrow \infty} V_{-g(m)} A^* V_{g(m)} \chi I = (A^g)^* \chi I$$

in  $\mathcal{L}(L^2(\mathbb{R}^n, \mathbb{C}^N), H^{-m}(\mathbb{R}^n, \mathbb{C}^N))$ . Here,

$$A^* u = \sum_{|\alpha| \leq m} D^\alpha (a_\alpha^* u) \quad \text{and} \quad (A^g)^* u = \sum_{|\alpha| \leq m} D^\alpha ((a_\alpha^g)^* u)$$

refer to the adjoint operators of  $A$ ,  $A_g : H^m(\mathbb{R}^n, \mathbb{C}^N) \rightarrow L^2(\mathbb{R}^n, \mathbb{C}^N)$ . Let finally  $\text{op}(A)$  denote the set of all limit operators of  $A$  obtained in this way.

**Theorem 2** *Let  $A$  be a uniformly elliptic differential operator of the form (2). Then  $A : H^m(\mathbb{R}^n, \mathbb{C}^N) \rightarrow L^2(\mathbb{R}^n, \mathbb{C}^N)$  is a Fredholm operator if and only if all limit operators of  $A$  are invertible as operators from  $H^m(\mathbb{R}^n, \mathbb{C}^N)$  to  $L^2(\mathbb{R}^n, \mathbb{C}^N)$ .*

**Proof.** Let  $(I - \Delta)^\alpha$  be the pseudodifferential operator with symbol  $(1 + |\xi|^2)^\alpha$ , and let  $A$  be a partial differential operator of the form (2). Then the operator  $B := A(I - \Delta)^{-m/2}$  belongs to the matrix Wiener algebra considered in [24]. It follows from results of [24] that  $B$ , considered as an operator from  $L^2(\mathbb{R}^n, \mathbb{C}^N)$  to  $L^2(\mathbb{R}^n, \mathbb{C}^N)$ , is a Fredholm operator if and only if all limit operators of  $B$  are invertible on  $L^2(\mathbb{R}^n, \mathbb{C}^N)$ . Since the limit operators  $B_g$  of  $B$  and  $A_g$  of  $A$  are related by the relation  $B_g = A_g(I - \Delta)^{-m/2}$  (which comes from the shift invariance of the operator  $\Delta$ ), the assertion follows. ■

The uniform ellipticity of the operator  $A$  implies the a priori estimate

$$\|u\|_{H^m(\mathbb{R}^n, \mathbb{C}^N)} \leq C (\|Au\|_{L^2(\mathbb{R}^n, \mathbb{C}^N)} + \|u\|_{L^2(\mathbb{R}^n, \mathbb{C}^N)}). \quad (4)$$

This estimate allows one to consider the uniformly elliptic differential operator  $A$  as a closed unbounded operator on  $L^2(\mathbb{R}^n, \mathbb{C}^N)$  with dense domain  $H^m(\mathbb{R}^n, \mathbb{C}^N)$ .

It turns out (see [3]) that  $A$ , considered as an unbounded operator in this way, is a (unbounded) Fredholm operator if and only if  $A$ , considered as a bounded operator from  $H^m(\mathbb{R}^n, \mathbb{C}^N)$  to  $L^2(\mathbb{R}^n, \mathbb{C}^N)$ , is a (common bounded) Fredholm operator.

We say that  $\lambda \in \mathbb{C}$  belongs to the *essential spectrum* of  $A$  if the operator  $A - \lambda I$  is not Fredholm as an unbounded differential operator. As above, we denote the essential spectrum of  $A$  by  $\text{sp}_{\text{ess}} A$  and the common spectrum of  $A$  (considered as an unbounded operator) by  $\text{sp} A$ . Then the assertion of Theorem 2 can be stated as follows.

**Theorem 3** *Let  $A$  be a uniformly elliptic differential operator of the form (2). Then*

$$\text{sp}_{\text{ess}} A = \bigcup_{A_g \in \text{op } A} \text{sp } A_g. \quad (5)$$

## 2.2 Exponential estimates

Let  $w$  be a positive measurable function on  $\mathbb{R}^n$ , which we call a weight. By  $L^2(\mathbb{R}^n, \mathbb{C}^N, w)$  we denote the space of all measurable functions on  $\mathbb{R}^n$  such that

$$\|u\|_{L^2(\mathbb{R}^n, \mathbb{C}^N, w)} := \|wu\|_{L^2(\mathbb{R}^n, \mathbb{C}^N)} < \infty.$$

In what follows we consider weights of the form  $w = \exp v$  where  $\partial_{x_j} v \in C_b^\infty(\mathbb{R}^n)$  for  $j = 1, \dots, n$  and

$$\lim_{x \rightarrow \infty} \partial_{x_i x_j}^2 v(x) = 0 \quad \text{for } 1 \leq i, j \leq n. \quad (6)$$

We call weights with these properties *slowly oscillating* and let  $\mathcal{R}$  stand for the class of all slowly oscillating weights.

Examples of slowly oscillating weights can be constructed as follows. Given a positive  $C^\infty$ -function  $l : S^{n-1} \rightarrow \mathbb{R}$ , set  $v_l(x) := l(x/|x|)|x|$ . Then  $w_l := \exp v_l$  defines a weight on  $\mathbb{R}^n$ . Clearly,  $v_l$  is a positively homogeneous function, that is  $v_l(tx) = tv_l(x)$  for all  $t > 0$  and  $x \in \mathbb{R}^n$ . Moreover,  $v_l \in C^\infty(\mathbb{R}^n \setminus \{0\})$ , and  $\nabla v_l(\omega) = l(\omega)\omega$  for every point  $\omega \in S^{n-1}$ . Let  $\tilde{v}_l$  refer to a  $C^\infty$ -function on  $\mathbb{R}^n$  which coincides with  $v_l$  outside a small neighborhood of the origin. Then the weight  $\tilde{w}_l := \exp \tilde{v}_l$  belongs to the class  $\mathcal{R}$ . Moreover,

$$\lim_{x \rightarrow \eta_\omega} \nabla \tilde{v}_l(x) = \nabla v_l(\omega) = l(\omega)\omega \quad (7)$$

for  $\omega \in S^{n-1}$ .

**Proposition 4** *Let  $A$  be a differential operator of the form (2), and let  $w = \exp v$  be a weight in  $\mathcal{R}$ . Then*

$$w^{-1}Aw = \sum_{|\alpha| \leq m} a_\alpha (D + i\nabla v)^\alpha + \Phi + R$$

where  $R := \sum_{|\alpha| \leq m-1} b_\alpha D^\alpha$  is a differential operator with continuous coefficients such that  $\lim_{x \rightarrow \infty} b_\alpha(x) = 0$ .

For a proof see [21] where a similar result is derived for a large class of pseudo-differential operators. The following is taken from [8], p. 308.

**Proposition 5** *Let  $X_1, X_2, Y_1$  and  $Y_2$  be Banach spaces such that  $X_1$  is densely embedded into  $X_2$  and  $Y_1$  is embedded into  $Y_2$ . Further let  $A : X_2 \rightarrow Y_2$  and  $A|_{X_1} : X_1 \rightarrow Y_1$  be Fredholm operators, and suppose that*

$$\text{ind}(A : X_2 \rightarrow Y_2) = \text{ind}(A|_{X_1} : X_1 \rightarrow Y_1).$$

*If  $u \in X_2$  is a solution of the equation  $Au = f$  with right-hand side  $f \in Y_1$ , then  $u \in X_1$ .*

**Theorem 6** *Let  $A$  be a uniformly elliptic differential operator of the form (2), and let  $w = \exp v$  be a weight in  $\mathcal{R}$  such that  $\lim_{x \rightarrow \infty} w(x) = +\infty$ . For  $t \in [-1, 1]$ , set*

$$A_{w,t} := \sum_{|\alpha| \leq m} a_\alpha (D + it\nabla v)^\alpha,$$

*and assume that*

$$0 \notin \bigcup_{t \in [-1, 1]} \text{sp}_{\text{ess}} A_{w,t} = \bigcup_{t \in [-1, 1]} \bigcup_{A_{w,t}^g \in \text{op}(A_{w,t})} \text{sp} A_{w,t}^g. \quad (8)$$

*If  $u$  is a function in  $H^m(\mathbb{R}^n, \mathbb{C}^N, w^{-1})$  for which  $Au$  is in  $L^2(\mathbb{R}^n, \mathbb{C}^N, w)$ , then  $u$  already belongs to  $H^m(\mathbb{R}^n, \mathbb{C}^N, w)$ .*

**Proof.** Note that  $A : H^m(\mathbb{R}^n, \mathbb{C}^N, w^t) \rightarrow L^2(\mathbb{R}^n, \mathbb{C}^N, w^t)$  is a Fredholm operator if and only if  $w^{-t}Aw^t : H^m(\mathbb{R}^n, \mathbb{C}^N) \rightarrow L^2(\mathbb{R}^n, \mathbb{C}^N)$  is a Fredholm operator, and that the Fredholm indices of these operator coincide. Proposition 4 implies that

$$w^{-t}Aw^t = \sum_{|\alpha| \leq m} a_\alpha (D + it\nabla v)^\alpha + R_t,$$

where  $R_t = \sum_{|\alpha| \leq m-1} b_{\alpha,t} D^\alpha$  and  $\lim_{x \rightarrow \infty} b_{\alpha,t}(x) = 0$  for every  $t \in [-1, 1]$ . Hence,  $\text{op}(w^{-t}Aw^t) = \text{op}(A_{w,t})$ . Moreover, it is not hard to see that the coefficients  $b_{\alpha,t}$  depend continuously on  $t \in [-1, 1]$ . Hence, the family  $w^{-t}Aw^t$  depends continuously on  $t$ , and condition (8) implies that all operators  $w^{-t}Aw^t : H^m(\mathbb{R}^n, \mathbb{C}^N) \rightarrow L^2(\mathbb{R}^n, \mathbb{C}^N)$  with  $t \in [-1, 1]$  are Fredholm operators and that the Fredholm indices of these operators coincide. This implies that each operator

$$A : H^m(\mathbb{R}^n, \mathbb{C}^N, w^t) \rightarrow L^2(\mathbb{R}^n, \mathbb{C}^N, w^t)$$

owns the Fredholm property and that the index of this operator is independent of  $t \in [-1, 1]$ . Since  $H^m(\mathbb{R}^n, \mathbb{C}^N, w)$  is densely embedded into  $H^m(\mathbb{R}^n, \mathbb{C}^N, w^{-1})$ , we can apply Proposition 5 to obtain that all solutions of the equation  $Au = f$  with right-hand side  $f \in L^2(\mathbb{R}^n, \mathbb{C}^N, w)$ , which a priori are in  $H^m(\mathbb{R}^n, \mathbb{C}^N, w^{-1})$ , in fact belong to  $H^m(\mathbb{R}^n, \mathbb{C}^N, w)$ . ■

**Corollary 7** *Let  $A$  be a uniformly elliptic differential operator of the form (2), and let  $w = \exp v$  be a weight in  $\mathcal{R}$  with  $\lim_{x \rightarrow \infty} w(x) = +\infty$ . Let  $\lambda \in \text{sp}_{dis} A$  and  $\lambda \notin \text{sp}_{ess} A_{tw}$  for all  $t \in [0, 1]$ . Then every eigenfunction of  $A$  associated with  $\lambda$  belongs to the space  $H^m(\mathbb{R}^n, \mathbb{C}^N, w)$ .*

Indeed, this is an immediate consequence of Theorem 6 since eigenfunctions of uniformly elliptic operator of order  $m$  necessarily belong to  $H^m(\mathbb{R}^n, \mathbb{C}^N)$ .

### 3 Schrödinger operators with matrix potentials

#### 3.1 Essential spectrum

We consider the Schrödinger operator

$$\mathcal{H} := (i\partial_{x_j} - a_j)\rho^{jk}(i\partial_{x_k} - a_k)E + \Phi \quad (9)$$

where  $E$  is the  $N \times N$  unit matrix,  $a = (a_1, \dots, a_n)$  is referred to as the magnetic potential, and  $\Phi = (\Phi_{pq})_{p,q=1}^N$  is a matrix potential on  $\mathbb{R}^n$ , the latter equipped with a Riemann metric  $\rho = (\rho_{jk})_{j,k=1}^n$  which is subject to the positivity condition

$$\inf_{x \in \mathbb{R}^n, \omega \in S^{n-1}} \rho_{jk}(x)\omega^j\omega^k > 0, \quad (10)$$

where  $\rho_{jk}(x)$  refers to the matrix inverse to  $\rho^{jk}(x)$ . Here and in what follows, we make use of Einstein's summation convention.

In what follows we suppose that  $\rho^{jk}$  and  $a_j$  are real-valued functions in  $SO^1(\mathbb{R}^n)$  and that  $\Phi_{pq} \in SO(\mathbb{R}^n)$ . Under these conditions,  $\mathcal{H}$  can be considered as a closed unbounded operator on  $L^2(\mathbb{R}^n, \mathbb{C}^N)$  with domain  $H^2(\mathbb{R}^n, \mathbb{C}^N)$ . If  $\Phi$  is a Hermitian matrix-valued function, then  $\mathcal{H}$  is a self-adjoint operator.

The limit operators of  $\mathcal{H}$  are the operators with constant coefficients

$$\mathcal{H}^g = (i\partial_{x_j} - a_j^g)\rho_g^{jk}(i\partial_{x_k} - a_k^g)E + \Phi^g$$

where

$$a^g := \lim_{m \rightarrow \infty} a(g_m), \quad \rho_g := \lim_{m \rightarrow \infty} \rho(g_m), \quad \Phi^g := \lim_{m \rightarrow \infty} \Phi(g_m). \quad (11)$$

The operator  $\mathcal{H}^g$  is unitarily equivalent to the operator

$$\mathcal{H}_1^g := -\rho_g^{jk}\partial_{x_j}\partial_{x_k}E + \Phi^g,$$

which on its hand is unitarily equivalent to the operator  $\widehat{\mathcal{H}_1^g}$  of multiplication by the matrix-function

$$\widehat{\mathcal{H}_1^g}(\xi) := (\rho_g^{jk}\xi_j\xi_k)E + \Phi^g$$



acting on  $L^2(\mathbb{R}^n, \mathbb{C}^N)$ . Evidently,

$$\text{sp } \widehat{\mathcal{H}}_1^g = \bigcup_{j=1}^N \Gamma_j^g$$

where  $\Gamma_j^g := \mu_j^g + \mathbb{R}$  and the  $\mu_j^g$ ,  $1 \leq j \leq N$ , run through the eigenvalues of the matrix  $\Phi^g$ . Thus, specifying (5) to the present context we obtain the following.

**Theorem 8** *The essential spectrum of the Schrödinger operator  $\mathcal{H}$  is given by*

$$\text{sp}_{ess} \mathcal{H} = \bigcup_g \bigcup_{j=1}^N \Gamma_j^g \quad (12)$$

where the union is taken with respect to all sequences  $g$  for which the limits in (11) exist.

The description (12) of the essential spectrum becomes much simpler if  $\Phi$  is a Hermitian matrix function, in which case  $\mathcal{H}$  is a self-adjoint operator.

**Theorem 9** *Let the potential  $\Phi$  be a Hermitian and slowly oscillating matrix function. Then*

$$\text{sp}_{ess} \mathcal{H} = [d_\Phi, +\infty)$$

where

$$d_\Phi := \liminf_{x \rightarrow \infty} \inf_{\|\varphi\|=1} \langle \Phi(x)\varphi, \varphi \rangle.$$

**Proof.** Since  $\Phi^g$  is Hermitian matrix,

$$\gamma_g := \inf_{\|\varphi\|=1} \langle \Phi^g \varphi, \varphi \rangle$$

is the smallest eigenvalue of  $\Phi^g$ . Hence,  $\text{sp } \mathcal{H}^g = [\gamma_g, +\infty)$  and, according to (5),

$$\text{sp}_{ess} \mathcal{H} = \bigcup_g [\gamma_g, +\infty) = [\inf_g \gamma_g, +\infty).$$

It remains to show that

$$\inf_g \gamma_g = d_\Phi. \quad (13)$$

Let  $g$  be a sequence tending to infinity for which the limit

$$\Phi^g := \lim_{m \rightarrow \infty} \Phi(g(m))$$

exists. Then, for each unit vector  $\varphi \in \mathbb{C}^N$ ,

$$\langle \Phi^g \varphi, \varphi \rangle = \lim_{m \rightarrow \infty} \langle \Phi(g(m))\varphi, \varphi \rangle \geq \liminf_{x \rightarrow \infty} \langle \Phi(x)\varphi, \varphi \rangle \geq d_\Phi,$$

whence  $\gamma_g \geq d_\Phi$ . For the reverse inequality, note that there exist a sequence  $g_0$  tending to infinity and a sequence  $\varphi$  in the unit sphere in  $\mathbb{C}^N$  with limit  $\varphi_0$  such that

$$d_\Phi = \lim_{m \rightarrow \infty} (\Phi(g_0(m))\varphi_m, \varphi_m) = (\Phi^{g_0}\varphi_0, \varphi_0) \geq \gamma_{g_0}.$$

Thus,  $\gamma_{g_0} = d_\Phi$ , whence (13). ■

### 3.2 Exponential estimates of eigenfunctions of the discrete spectrum

Here we suppose that the components  $\rho^{jk}$  of the Riemann metric, the coefficients  $a_\alpha$  and the weight  $w$  are slowly oscillating functions and that  $\Phi$  is a Hermitian slowly oscillating matrix function. Every limit operator  $(w^{-1}\mathcal{H}w)_g$  of  $w^{-1}\mathcal{H}w$  is unitarily equivalent to the operator

$$\mathcal{H}_w^g := \rho_g^{jk}(D_{x_j} + i(\nabla v)_j^g)(D_{x_k} + i(\nabla v)_k^g) + \Phi^g E,$$

where  $\rho_g^{jk}$  and  $\Phi^g$  are the limits defined by (11) and

$$(\nabla v)^g := \lim_{k \rightarrow \infty} (\nabla v)(g(k)) \in \mathbb{R}^n. \quad (14)$$

We set

$$|(\nabla v)|_\rho^2 := \rho^{jk}(\nabla v)_j(\nabla v)_k \quad \text{and} \quad |(\nabla v)^g|_{\rho_g}^2 := \rho_g^{jk}(\nabla v)_j^g(\nabla v)_k^g.$$

The operator  $\mathcal{H}_w^g$  is unitarily equivalent to the operator of multiplication by the matrix-valued function

$$\widehat{\mathcal{H}_w^g}(\xi) := \rho_g^{jk}(\xi_j + i(\nabla v)_j^g)(\xi_k + i(\nabla v)_k^g) + \Phi^g E, \quad \xi \in \mathbb{R}^n,$$

the real part of which is

$$\Re(\widehat{\mathcal{H}_w^g}) = \rho_g^{jk} \xi_j \xi_k + (\Phi^g - |(\nabla v)^g|_{\rho_g}^2 E). \quad (15)$$

Corollary 7 implies the following.

**Theorem 10** *Let  $\lambda \in \text{sp}_{dis} \mathcal{H}$ , and let  $w = \exp v$  be a weight in  $\mathcal{R}$  for which*

$$\limsup_{x \rightarrow \infty} |(\nabla v)(x)|_{\rho(x)} < \sqrt{d_\Phi - \lambda}.$$

*Then every  $\lambda$ -eigenfunction of  $\mathcal{H}$  belongs to  $H^2(\mathbb{R}^n, w)$ .*

**Corollary 11** *Let  $\lambda \in \text{sp}_{dis} \mathcal{H}$ , and let  $c \in \mathbb{R}$  satisfy*

$$0 < c < \frac{\sqrt{d_\Phi - \lambda}}{\rho^{\text{sup}}}$$

*where*

$$\rho^{\text{sup}} := \liminf_{x \rightarrow \infty} \sup_{\omega \in S^{n-1}} (\rho^{jk}(x) \omega_j \omega_k)^{1/2}.$$

*Then the every  $\lambda$ -eigenfunction of  $\mathcal{H}$  belongs to the space  $H^2(\mathbb{R}^n, \mathbb{C}^N, w)$  with weight  $w(x) = e^{c\langle x \rangle}$ .*

## 4 Quaternionic operators

We let  $\mathbb{H}(\mathbb{C})$  denote the complex quaternionic algebra, which is the associative algebra over the field  $\mathbb{C}$  of complex numbers generated by four elements  $1, e_1, e_2, e_3$  subject to the conditions

$$e_1e_2 = e_3, \quad e_2e_3 = e_1, \quad e_3e_1 = e_2$$

and

$$1^2 = 1, \quad e_k^2 = -1, \quad 1e_k = e_k1 = e_k, \quad e_je_k = -e_ke_j$$

for  $j, k = 1, 2, 3$ . Each of the elements  $1, e_1, e_2, e_3$  commutes with the imaginary unit  $i$ . Hence, every element  $q \in \mathbb{H}(\mathbb{C})$  has a unique decomposition

$$q = q_0 + q_1e_1 + q_2e_2 + q_3e_3 =: q_0 + \mathbf{q}$$

with complex numbers  $q_j$ . The number  $q_0$  is called the scalar part of the quaternion  $q$ , and  $\mathbf{q}$  is its vector part. One can also think of  $\mathbb{H}(\mathbb{C})$  as a complex linear space of dimension four with usual linear operations. With respect to the base  $\{1, e_1, e_2, e_3\}$  of this space, the operator of multiplication by 1 has the unit matrix  $E_4$  as its matrix representation, whereas the matrix representations  $\gamma_j$  of the operators of multiplication by  $e_j$ ,  $j = 1, 2, 3$ , are real and skew-symmetric, that is  $\gamma_j^t = -\gamma_j$ . The space  $\mathbb{H}(\mathbb{C})$  carries also the structure of a complex Hilbert space via the scalar product

$$\langle q, r \rangle_{\mathbb{H}(\mathbb{C})} := q_0\bar{r}_0 + q_1\bar{r}_1 + q_2\bar{r}_2 + q_3\bar{r}_3.$$

By  $L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$  we denote the Hilbert space of all measurable and squared integrable quaternion-valued functions on  $\mathbb{R}^3$  which is provided with the scalar product

$$\langle u, v \rangle_{L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))} := \int_{\mathbb{R}^3} \langle u(x), v(x) \rangle_{\mathbb{H}(\mathbb{C})} dx.$$

In a similar way, we introduce the quaternionic Sobolev space  $H^1(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$ . Further we write  $M^\varphi$  for the operator of multiplication from the right by the complex quaternionic function  $\varphi$ , that is

$$(M^\varphi u)(x) = u(x)\varphi(x) \quad \text{for } x \in \mathbb{R}^3.$$

Clearly, if  $\varphi \in L^\infty(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$ , then  $M^\varphi$  acts as a bounded linear operator on  $L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$ .

Differential operators of the form

$$A(x, D)u(x) := \sum_{j=1}^3 a_j(x)D_{x_j}e_ju(x) + M^{\varphi(x)}u(x), \quad x \in \mathbb{R}^3, \quad (16)$$

can be considered as generalized Moisil-Theodorescu operators. Note that each operator of the form (16) corresponds to a matrix operator with respect to the basis  $\{1, e_1, e_2, e_3\}$ . It has been pointed out in [9, 11, 12] that some of the

most popular operators of mathematical physics, including Dirac and Maxwell operators, are of the form (16).

In this section, we suppose that the coefficients  $a_j$  belong to  $SO^1(\mathbb{R}^3)$  and satisfy

$$\inf_{x \in \mathbb{R}^3} |a_j(x)| > 0 \quad \text{for } j = 1, 2, 3 \quad (17)$$

and that the components  $\varphi_k$  of  $\varphi$  belong to  $SO(\mathbb{R}^3)$ .

The main symbol of the operator  $A$  is

$$A_0(x, \xi) = \sum_{j=1}^3 a_j(x) (i\xi_j) e_j.$$

Hence,

$$A_0^2(x, \xi) = \sum_{j=1}^3 a_j^2(x) \xi_j^2$$

is a scalar function, and from (17) we conclude that the associated operator  $A_0$  is uniformly elliptic on  $\mathbb{R}^3$ .

**Theorem 12** *The quaternionic operator  $A(x, D)$  thought of as acting from  $H^1(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$  to  $L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$  is a Fredholm operator if and only if*

$$\liminf_{x \rightarrow \infty} \left| A_0^2(x, \xi) + \sum_{j=1}^3 \varphi_j(x)^2 \right| > 0 \quad \text{for every } \xi \in \mathbb{R}^3. \quad (18)$$

**Proof.** The limit operators of  $A(x, D)$  are the operators with constant coefficients

$$A^g(D)u := \sum_{j=1}^3 a_j^g D_{x_j} e_j u + M^{\varphi^g} u.$$

Let  $\check{A}^g(D) := \sum_{j=1}^3 a_j^g D_{x_j} e_j - M^{\varphi^g}$ . Then

$$A^g(D)\check{A}^g(D) = - \sum_{j=1}^3 (a_j^g)^2 D_{x_j}^2 - (\varphi^g)^2$$

where

$$-(\varphi^g)^2 = (\varphi_1^g)^2 + (\varphi_2^g)^2 + (\varphi_3^g)^2.$$

Condition (17) implies that  $A^g(D) : H^1(\mathbb{R}^3, \mathbb{H}(\mathbb{C})) \rightarrow L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$  is an invertible operator if and only if

$$\inf_{\xi \in \mathbb{R}^n} \left| (A_0^g)^2(\xi) + \sum_{j=1}^3 (\varphi_j^g)^2 \right| > 0 \quad \text{for every } \xi \in \mathbb{R}^3. \quad (19)$$

Hence, all limit operators  $A^g(D)$  of  $A(D)$  are invertible as operators from  $H^1(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$  to  $L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$  if and only if condition (18) holds.  $\blacksquare$

**Theorem 13** *In addition to the above assumptions, let all functions  $a_j$  and  $\varphi_j$  be real-valued, and let  $w = \exp v$  be a weight in  $\mathcal{R}$  with  $\lim_{x \rightarrow \infty} v(x) = +\infty$ . If the condition*

$$\liminf_{x \rightarrow \infty} \left( \sum_{j=1}^3 \varphi_j^2(x) - a_j^2(x) \left( \frac{\partial v(x)}{\partial x_j} \right)^2 \right) > 0 \quad (20)$$

*is satisfied, then every solution  $u \in H^1(\mathbb{R}^3, \mathbb{H}(\mathbb{C}), w^{-1})$  of the equation  $Au = f$  with right-hand side  $f \in L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}), w)$  belongs to  $H^1(\mathbb{R}^3, \mathbb{H}(\mathbb{C}), w)$ .*

**Proof.** Let  $t \in [-1, 1]$ . The limit operators of  $A_{w,t}(x, D)$  are operators with constant coefficients of the form

$$A_{w,t}^g(D) = \sum_{j=1}^3 a_j^g(D_{x_j} + it \left( \frac{\partial v}{\partial x_j} \right)^g) e_j + M^{\varphi^g}.$$

As above, let

$$\check{A}_{w,t}^g(D) := \sum_{j=1}^3 a_j^g(D_{x_j} + it \left( \frac{\partial v}{\partial x_j} \right)^g) e_j - M^{\varphi^g}.$$

Then  $A_{w,t}^g(D) \check{A}_{w,t}^g(D)$  is a scalar operator with symbol

$$A_{w,t}^g(\xi) \check{A}_{w,t}^g(\xi) = \sum_{j=1}^3 (a_j^g)^2 (\xi_j + it \left( \frac{\partial v}{\partial x_j} \right)^g)^2 + \sum_{j=1}^3 (\varphi_j^g)^2(x),$$

the real part of which is

$$\Re(A_{w,t}^g(\xi) \check{A}_{w,t}^g(\xi)) = \sum_{j=1}^3 (a_j^g)^2 \xi_j^2 + \sum_{j=1}^3 (\varphi_j^g)^2 - t^2 \left[ \left( \frac{\partial v}{\partial x_j} \right)^g \right]^2.$$

Condition (20) implies that

$$A_{w,t}^g(\xi) \check{A}_{w,t}^g(\xi) \neq 0 \quad (21)$$

for every  $\xi \in \mathbb{R}^3$  and  $t \in [-1, 1]$ . Without change of notation, we now consider  $A_{w,t}^g(\xi)$  as a  $4 \times 4$  matrix-valued function. The matrix  $A_{w,t}^g(\xi)$  is invertible for every  $\xi \in \mathbb{R}^3$  and  $t \in [-1, 1]$  and for every sequence  $g$  which defines a limit operator. Together with condition (17), this fact implies that  $A_{w,t}^g(D) : H^1(\mathbb{R}^3, \mathbb{H}(\mathbb{C})) \rightarrow L^2(\mathbb{R}^3, \mathbb{H}(\mathbb{C}))$  is an invertible operator for every  $t \in [-1, 1]$  and for every sequence  $g$  which defines a limit operator. Hence, Theorem 13 is a consequence of Corollary 7.  $\blacksquare$

## 5 Dirac operators

### 5.1 Essential spectrum of Dirac operators

In this section we consider the Dirac operator on  $\mathbb{R}^3$  equipped with the Riemann metric tensor  $(\rho_{jk})$  depending on  $x \in \mathbb{R}^3$  (see for instance [30]). We suppose

that there is a constant  $C > 0$  such that

$$\rho_{jk}(x)\xi^j\xi^k \geq C|\xi|^2 \quad \text{for every } x \in \mathbb{R}^3 \quad (22)$$

where we use the Einstein summation convention again. Let  $\rho^{jk}$  be the tensor inverse to  $\rho_{jk}$ , and let  $\phi^{jk}$  be the positive square root of  $\rho^{jk}$ . The Dirac operator on  $\mathbb{R}^3$  is the operator

$$\mathcal{D} := \frac{c}{2}\gamma_k(\phi^{jk}P_j + P_j\phi^{jk}) + \gamma_0c^2m - e\Phi \quad (23)$$

acting on functions on  $\mathbb{R}^3$  with values in  $\mathbb{C}^4$ . In (23), the  $\gamma_k$ ,  $k = 0, 1, 2, 3$ , are the  $4 \times 4$  Dirac matrices, i.e., they satisfy

$$\gamma_j\gamma_k + \gamma_k\gamma_j = 2\delta_{jk}E \quad (24)$$

for all choices of  $j, k = 0, 1, 2, 3$  where  $E$  is the  $4 \times 4$  unit matrix,

$$P_j = D_j + \frac{e}{c}A_j, \quad D_j = \frac{h}{i}\frac{\partial}{\partial x_j}, \quad j = 1, 2, 3,$$

where  $h$  is the Planck constant,  $\vec{A} = (A_1, A_2, A_3)$  is the vector potential of the magnetic field  $\vec{H}$ , that is  $\vec{H} = \text{rot } \vec{A}$ ,  $\Phi$  is the scalar potential of the electric field  $\vec{E}$ , that is  $\vec{E} = \text{grad } \Phi$ , and  $m$  and  $e$  are the mass and the charge of the electron.

We suppose that  $\rho^{jk}$ ,  $A_j$  and  $\Phi$  are real-valued functions which satisfy the conditions

$$\rho^{jk} \in SO^1(\mathbb{R}^3), \quad A_j \in SO^1(\mathbb{R}^3), \quad \Phi \in SO(\mathbb{R}^3) \quad (25)$$

for  $j, k = 1, 2, 3$ . We consider the operator  $\mathcal{D}$  as an unbounded operator on the Hilbert space  $L^2(\mathbb{R}^3, \mathbb{C}^4)$  with domain  $H^1(\mathbb{R}^3, \mathbb{C}^4)$ . The conditions imposed on the magnetic and electric potentials  $\vec{A}$  and  $\Phi$  guarantee the self-adjointness of  $\mathcal{D}$ . The main symbol of  $\mathcal{D}$  is

$$a_0(x, \xi) = c\phi^{jk}(x)\xi_j\gamma_k.$$

Using (24) and the identity  $\phi^{jk}(x)\phi^{rt}(x)\delta_{kt} = \rho^{jr}(x)$  we obtain

$$\begin{aligned} a_0(x, \xi)^2 &= c^2h^2\phi^{jk}(x)\phi^{rt}(x)\xi_j\xi_r\gamma_k\gamma_t \\ &= c^2h^2\phi^{jk}(x)\phi^{rt}(x)\delta_{kt}\xi_j\xi_r \\ &= c^2h^2\rho^{jr}(x)\xi_j\xi_rE. \end{aligned} \quad (26)$$

Together with (22) this equality shows that  $\mathcal{D}$  is a uniformly elliptic differential operator on  $\mathbb{R}^3$ .

Conditions (25) imply that limit operators  $\mathcal{D}_g$  of  $\mathcal{D}$  defined by the sequences  $g : \mathbb{N} \rightarrow \mathbb{Z}^3$  tending to infinity are operators with constant coefficients of the form

$$\mathcal{D}_g = c\gamma_k\phi_q^{jk}(D_j + \frac{e}{c}A_j^g) + \gamma_0mc^2 - e\Phi^g \quad (27)$$

where

$$\phi_g^{jk} := \lim_{m \rightarrow \infty} \phi^{jk}(g(m)), \quad A_j^g := \lim_{m \rightarrow \infty} A_j(g(m)), \quad \Phi^g := \lim_{m \rightarrow \infty} \Phi(g(m)). \quad (28)$$

Note that one can suppose without loss of generality that the sequence  $g$  is such that the limits in (28) exist. In the opposite case we pass to a suitable subsequence of  $g$ .

The operator  $\mathcal{D}_g$  is unitarily equivalent to the operator

$$\mathcal{D}_g^1 = c\gamma_l \omega_g^{jl} D_j + \gamma_0 m c^2 - e\Phi^g,$$

and the equivalence is realized by the unitary operator

$$T_{\vec{A}^g} : f \mapsto e^{i\frac{e}{c}\vec{A}^g \cdot x} f \quad \text{where} \quad \vec{A}^g := (A_1^g, A_2^g, A_3^g).$$

Let

$$\Phi^{\text{sup}} := \limsup_{x \rightarrow \infty} \Phi(x), \quad \Phi^{\text{inf}} := \liminf_{x \rightarrow \infty} \Phi(x).$$

Then the interval  $[\Phi^{\text{inf}}, \Phi^{\text{sup}}]$  is just the set of all partial limits  $\Phi^g$  of function  $\Phi$  as  $x \rightarrow \infty$ .

**Theorem 14** *Let conditions (25) be fulfilled. Then the Dirac operator*

$$\mathcal{D} : H^1(\mathbb{R}^3, \mathbb{C}^4) \rightarrow L^2(\mathbb{R}^3, \mathbb{C}^4)$$

*is a Fredholm operator if and only if*

$$[\Phi^{\text{inf}}, \Phi^{\text{sup}}] \subset (-m c^2/e, m c^2/e). \quad (29)$$

**Proof.** Set  $\mathcal{D}_0^g(\xi) := c h \gamma_k \phi_g^{jk} \xi_j + \gamma_0 m c^2$  and  $\rho_j^{jk} := \lim_{m \rightarrow \infty} \rho^{jk}(g_m)$ . Then

$$\begin{aligned} & (\mathcal{D}_0^g(\xi) - e\Phi_1^g E)(\mathcal{D}_0^g(\xi) + e\Phi^g E) \\ &= (c^2 h^2 \rho_g^{jk} \xi_j \xi_k + m^2 c^4 - (e\Phi^g)^2) E. \end{aligned} \quad (30)$$

Let condition (29) be fulfilled. Then every partial limit  $\Phi^g = \lim_{k \rightarrow \infty} \Phi(g(k))$  of  $\Phi$  lies in the interval  $(-m c^2/e, m c^2/e)$ . The identity (30) implies that

$$\det(\mathcal{D}_0^g(\xi) - e\Phi^g E) \neq 0$$

for every  $\xi \in \mathbb{R}^3$ . Hence, the operator  $\mathcal{D}_g^1 : H^1(\mathbb{R}^3, \mathbb{C}^4) \rightarrow L^2(\mathbb{R}^3, \mathbb{C}^4)$  is invertible and, consequently, so is  $\mathcal{D}_g$ . By Theorem 2,  $\mathcal{D}$  is a Fredholm operator.

For the reverse implication, assume that condition (29) is not fulfilled. Then there exist a number  $\Phi^g \notin (-m c^2/e, m c^2/e)$  and a vector  $\xi^0 \in \mathbb{R}^3$  such that

$$c^2 g_g^{jk} \xi_j^0 \xi_k^0 + m^2 c^4 - (e\Phi^g)^2 = 0.$$

Given  $\xi^0$  we find a vector  $u \in \mathbb{C}^4$  such that  $v := (\mathcal{D}_0^g(\xi^0) + (e\Phi^g)E)u \neq 0$ . Then (30) implies that

$$(\mathcal{D}_0^g(\xi^0) - e\Phi^g E)v = 0,$$

whence

$$\det(\mathcal{D}_0^g(\xi^0) - e\Phi^g E) = 0.$$

Thus, the operator  $\mathcal{D}_g$  is not invertible. By Theorem 2,  $\mathcal{D}$  cannot be a Fredholm operator.  $\blacksquare$

**Theorem 15** *If condition (25) is satisfied, then*

$$\text{sp}_{ess} \mathcal{D} = (-\infty, -e\Phi^{\text{inf}} - mc^2] \cup [-e\Phi^{\text{sup}} + mc^2, +\infty).$$

**Proof.** Let  $\lambda \in \mathbb{C}$ . The symbol of the operator  $\mathcal{D}_g - \lambda I$  is the function  $\xi \mapsto \mathcal{D}_0^g(\xi) - (e\Phi^g + \lambda)E$ . Invoking (30) we obtain

$$\begin{aligned} & (\mathcal{D}_0^g(\xi) - (e\Phi^g + \lambda)E)(\mathcal{D}_0^g(\xi) + (e\Phi^g + \lambda)E) \\ &= (c^2 \rho_g^{jk} \xi_j \xi_k + m^2 c^4 - (e\Phi^g + \lambda)^2) E. \end{aligned} \quad (31)$$

Repeating the arguments from the proof of Theorem 14, we find that the eigenvalues  $\lambda_{\pm}^g(\xi)$  of the matrix  $\mathcal{D}_0^g(\xi) - e\Phi_1^g E$  are given by

$$\lambda_{\pm}^g(\xi) := -e\Phi^g \pm (c^2 \rho_g^{jk} \xi_j \xi_k + m^2 c^4)^{1/2}. \quad (32)$$

From (32) we further conclude

$$\begin{aligned} \{\lambda \in \mathbb{R} : \lambda = \lambda_-^g(\xi), \xi \in \mathbb{R}^3\} &= (-\infty, -e\Phi^g - mc^2], \\ \{\lambda \in \mathbb{R} : \lambda = \lambda_+^g(\xi), \xi \in \mathbb{R}^3\} &= [-e\Phi^g + mc^2, +\infty). \end{aligned}$$

Hence,

$$\text{sp} \mathcal{D}^g = (-\infty, -e\Phi^g - mc^2] \cup [-e\Phi^g + mc^2, +\infty),$$

whence the assertion via Theorem 3.  $\blacksquare$

Thus, if  $\Phi^{\text{sup}} - \Phi^{\text{inf}} \geq 2mc^2/e$ , then  $\text{sp}_{ess} \mathcal{D}$  is all of  $\mathbb{R}$ , whereas  $\text{sp}_{ess} \mathcal{D}$  has a proper gap in the opposite case.

## 5.2 Exponential estimates of eigenfunctions of the Dirac operator

**Theorem 16** *Let the conditions (25) be fulfilled. Let  $\lambda$  be an eigenvalue of  $\mathcal{D}$  which lies in the gap  $(-e\Phi^{\text{inf}} - mc^2, -e\Phi^{\text{sup}} + mc^2)$  of the essential spectrum. Further, let  $w = \exp v$  be a weight in  $\mathcal{R}$  with  $\lim_{x \rightarrow \infty} w(x) = \infty$  which satisfies*

$$\limsup_{x \rightarrow \infty} |\nabla v(x)|_{\rho(x)} < \frac{1}{c\hbar} \sqrt{m^2 c^4 - (e\Phi^{\text{sup}} + \lambda)^2}. \quad (33)$$

*Then every eigenfunction of  $\mathcal{D}$  associated with  $\lambda$  belongs to  $H^1(\mathbb{R}^3, \mathbb{C}^4, w)$ .*

**Proof.** Let  $\lambda \in (-e\Phi^{\text{inf}} - mc^2, -e\Phi^{\text{sup}} + mc^2)$  be an eigenvalue of  $\mathcal{D}$ . As above, we examine the spectra of the limit operators  $(\mathcal{D}_{w,t})_g$  of  $\mathcal{D}_{w,t} := w^{-t} \mathcal{D} w^t$  for  $t$  running through  $[0, 1]$ . Let  $(\mathcal{D}_{w,t})_g$  be a limit operator of  $\mathcal{D}_{w,t}$  with respect to a sequence  $g$  tending to infinity. One easily checks that  $(\mathcal{D}_{tw})_g$  is unitarily equivalent to the operator

$$(\mathcal{D}'_{tw})_g := A_{t,g} - e\Phi^g E$$



where

$$A_{t,g} := c\gamma_k \phi_g^{jk} (D_j + ith(\frac{\partial v}{\partial x_j})^g) + \gamma_0 m c^2.$$

The operator  $A_{t,g}$  has constant coefficients, and its symbol is

$$\widehat{A_{t,g}}(\xi) = c\gamma_k \phi_g^{jk} (h(\xi_j + ith(\frac{\partial v}{\partial x_j})^g)) + \gamma_0 m c^2.$$

Further,

$$\begin{aligned} & \Re \left[ \left( \widehat{A_{t,g}}(\xi) - (e\Phi^g - \lambda)E \right) \left( \widehat{A_{t,g}}(\xi) + (e\Phi^g - \lambda)E \right) \right] \\ &= \Re \left[ c^2 h^2 \rho_g^{jk} \left( \xi_j + ith(\frac{\partial v}{\partial x_j})^g \right) \left( \xi_k + ith(\frac{\partial v}{\partial x_k})^g \right) \right] \\ & \quad + \Re \left[ (m^2 c^4 - (e\Phi^g + \lambda)^2) E \right] \\ &= \left[ c^2 h^2 \rho_g^{jk} \xi_j \xi_k - c^2 h^2 t^2 \rho_g^{jk} \left( \frac{\partial v}{\partial x_j} \right)^g \left( \frac{\partial v}{\partial x_k} \right)^g + (m^2 c^4 - (e\Phi^g + \lambda)^2) \right] E \\ &=: \gamma_{g,t}(\xi, \lambda) E. \end{aligned}$$

Assume that condition (33) is fulfilled. Then, since  $c^2 h^2 \rho_g^{jk} \xi_j \xi_k \geq 0$ ,

$$\inf_{\xi \in \mathbb{R}^n} \gamma_{g,t}(\xi, \lambda) > 0$$

for all  $t \in [0, 1]$  and for all sequences  $g \rightarrow \infty$  for which the limit operators exist. Hence, (33) implies that the matrix  $\widehat{A_{t,g}}(\xi) - (e\Phi^g - \lambda)E$  is invertible for every  $\xi \in \mathbb{R}^3$ . On the other hand, due to the uniform ellipticity of  $A_{t,g}$  one has  $\lambda \in \text{sp} \left( \widehat{A_{t,g}}(\xi) - (e\Phi^g - \lambda)E \right)$  if and only if there exists a  $\xi_0 \in \mathbb{R}^3$  such that the matrix  $\widehat{A_{t,g}}(\xi_0) - (e\Phi^g + \lambda)E$  is not invertible. Thus,  $\lambda \notin \text{sp}(\mathcal{D}_{tw})_g$  for every  $t \in [0, 1]$  and every sequence  $g \rightarrow \infty$ . Via Corollary 7, the assertion follows. ■

We conclude by an example. Let the conditions (25) be fulfilled, and let  $\lambda$  be an eigenvalue of  $\mathcal{D}$  in  $(-e\Phi^{\text{inf}} - mc^2, -e\Phi^{\text{sup}} + mc^2)$  and  $u_\lambda$  an associated eigenfunction. If  $a$  satisfies the estimates

$$0 < a < \frac{\sqrt{m^2 c^4 - (e\Phi^{\text{sup}} + \lambda)^2}}{ch\rho^{\text{sup}}}$$

where

$$\rho^{\text{sup}} := \liminf_{x \rightarrow \infty} \sup_{\omega \in S^2} (\rho^{jk}(x) \omega_j \omega_k)^{1/2},$$

then  $u_\lambda \in H^1(\mathbb{R}^3, \mathbb{C}^4, e^{a\langle x \rangle})$ .

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