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ON A DOMAIN OPTIMIZATION PROBLEM FOR THE PAULI OPERATOR

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Abstract. In the paper a minimization problem is considered for the eigenvalues of Pauli operator. The domain of the operator is assumed variable and as a result the eigenvalues are studied as a domain functional. A minimization problem for the first eigenvalue is formulated with respect to domain. Using the formula obtained for the first variation of the eigenvalues a numerical algorithm is proposed for the solution of the considered problem.

Keywords: Pauli operator, domain functional, shape optimization, eigenvalue, numerical algorithm.

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1. Introduction

We study the eigenvalues of Pauli operator. It is known that the operator Pauli describes the motion of a particle with spin (as opposed to the Schrödinger operator) in a magnetic field, and is a generalization of the Schrödinger operator in mathematical and quantum-physical senses [3]. Inside angular momentum of a particle, which has been shown in the Stern-Gerlach experiment, is called a spin. We are talking about angular momentum of the particle, even when it is completely at rest. In quantum physics, it is shown that the particle can have a spin that is not associated with the movement of its parts with respect to the center of mass. In particular, the real elementary particle (which has no internal components) may also possess spin [12]. Therefore Pauli operator has a wide application in quantum physics. As follows from the basic postulates of quantum physics, the eigenvalues λ_n of Pauli operator describe the total energy of the quantum system (in our case the electron with spin in the magnetic field) in the state φ_n, where φ_n is an eigenfunction of Pauli operator corresponding to the eigenvalue λ_n [3]. In this paper, we assume that the domain of definition of the operator variable. In such a case, and a private function φ_n (i.e. the state of a quantum system) and the corresponding eigenvalue λ_n are functionals of the field. Studying the behavior of the quantum-mechanical values when the domain varies is an important problem, both from theoretical and practical points of view. We study the eigenvalues of Pauli operator in the variable operator definition domain.

2. Preliminary facts and background

A number of works have been devoted to the investigation of the various shape optimization (optimization with respect to domain) problems for the eigenvalues of different operators. The main problem here is that the argument of the functionals under minimization is a domain. This is the principle difference of the shape optimization problems from the traditional ones. This fact leads the researchers to the necessity to develop new approaches for investigation of these problems. One of the methods was introduced by Cea J. and developed by Sokołowski and J.-P. Zolesio and is called vector filed method [7]. In spite of this method gives possibility to solve a wide class of problems, there exists a class of problems out of responsibility of this method.

To cover wider front of the studied problems in [12] a new definition of the domain variation is introduced using one-to-one mapping between bounded convex sets and continuous positive homogeneous convex functions was offered.

The method is mainly based on the expression of the variation of the convex bounded domains by the variation of its support function. Using this fact a shape derivative formula is derived for the integral cost functional in the class of bounded convex domains [12].

This approach allows one to avoid some of disadvantages of the existing methods [7]. For instance applying this method in the process of numerical simulation after next iteration we get not only a set of boundary points, but also the values of the support function. The domain then is reconstructed as a sub-differential of its support function in the point 0.

Note that this approach has been extended for more large classes of metrics and functions by other authors. For instance in [2] the shape derivative formula for the integral cost functional with respect to a class of admissible convex domains given in [12] is extended to the case of $W^{1,1}_{loc}$ functions are implemented in Brunn-Minkowski theory.

Now we give the definition of the variation of the functional in the space ML_2 referring to [12]. As in [12] let's denote $M = \{D \in R^n : S_D \in C^2\}$.

The functional $\lambda(D)$ is called differentiable in the Gateaux sense on M in the direction K_0 if for any $D \in M$ there exists the limit

$$\delta\lambda(D_0, D) = \lim_{\varepsilon \to +0} \frac{\lambda((1-\varepsilon)D_0 + \varepsilon D) - \lambda(D_0)}{\varepsilon}. \qquad (1)$$

Let Ω be the set of all convex bounded closed domains from R^2 with smooth boundaries. Denote

$$K = \{D \in \Omega,\ \ \overline{D} \in \Omega_0,\ \ S_D \in C^2\}, \qquad (2)$$

where Ω_0 is some convex subset of Ω, $\overline{D}$ is a closure and S_D - boundary of the domain D.

3. Problem formulation and main results

Consider the problem

$$J(D) = \lambda_1(D) + \int_D f(x)dx \to \min, \quad D \in K, \tag{3}$$

where $f(x)$ is a given integrable function, λ_1 is the first eigenvalue of the following spectral problem

$$P\varphi = \lambda\varphi, \qquad x \in D, \tag{8}$$

$$\varphi = 0, \qquad x \in S_D, \tag{9}$$

where P is Pauli operator generated by the expression

$$P = P(a,v)\cdot J + \sigma B. \tag{10}$$

Here

$$J = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad P = (a,v) = (-i\nabla - a)^2 + V,$$

i is the imaginary unit, V is a smooth enough function, $\nabla = \left\{\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right\}$, $a = (a_1, a_2) \in R^2$ is a vector potential, B - magnetic field generated by a, i.e. $B = \frac{\partial}{\partial x}a_2 - \frac{\partial}{\partial y}a_1$.

If to consider these definitions in (10) one can obtain the following explicit form of two dimensional Pauli operator

$$P = \begin{pmatrix} (-i\nabla - a)^2 + a_2\frac{\partial}{\partial x} - a_1\frac{\partial}{\partial y} + V & 0 \\ 0 & (-i\nabla - a)^2 - a_2\frac{\partial}{\partial x} + a_1\frac{\partial}{\partial y} + V \end{pmatrix} =$$

$$= \begin{pmatrix} -\Delta + (2ia_1 + a_2)\frac{\partial}{\partial x} + (2ia_2 - a_1)\frac{\partial}{\partial y} + a^2 + V & 0 \\ 0 & -\Delta + (2ia_1 - a_2)\frac{\partial}{\partial x} + (2ia_2 + a_1)\frac{\partial}{\partial y} + a^2 + V \end{pmatrix}. \tag{5}$$

Taking $\varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$, where $\varphi_1, \varphi_2 \in L_2(D)$ from (2) and (5) we get

$$\begin{aligned} -\Delta\varphi_1 + (2ia_1 + a_2)\frac{\partial\varphi_1}{\partial x} + (2ia_2 - a_1)\frac{\partial\varphi_1}{\partial y} + a^2\varphi_1 + V\varphi_1 = \lambda\varphi_1, \\ -\Delta\varphi_2 + (2ia_1 - a_2)\frac{\partial\varphi_2}{\partial x} + (2ia_2 + a_1)\frac{\partial\varphi_2}{\partial y} + a^2\varphi_2 + V\varphi_2 = \lambda\varphi_2. \end{aligned} \tag{6}$$

Denote

$$P_1 = -\Delta + (2ia_1 + a_2)\frac{\partial}{\partial x} + (2ia_2 - a_1)\frac{\partial}{\partial y} + a^2 + V,$$

$$P_2 = -\Delta + (2ia_1 - a_2)\frac{\partial}{\partial x} + (2ia_2 + a_1)\frac{\partial}{\partial y} + a^2 + V .$$

Thus within some conditions on a we can consider eigenvalues of Pauli operator positive and numerated in increasing order considering their multiplicity $0 \le \lambda_1 \le \lambda_2 \le \dots$.

Replacing $\varphi_i' = e^{\alpha x + \beta y}\varphi_i$, $i = 1,2$, $\alpha,\ \beta \in R$ after some transformations (6) we get

$$-\Delta\varphi_1 + V\varphi_1 = \left(\lambda - \frac{1}{4}a^2\right)\varphi_1 , \tag{7}$$

$$-\Delta\varphi_2 + V\varphi_2 = \left(\lambda - \frac{1}{4}a^2\right)\varphi_2 . \tag{8}$$

Taking $\eta = \lambda - \frac{1}{4}a^2$ from (5), (7), (8) we can rewrite the problem (2), (3) in the form

$$\begin{aligned} \tilde{P}\varphi &= \eta\varphi, \quad x \in D, \\ \varphi &= 0 \quad , \quad x \in S_D , \end{aligned} \tag{9}$$

where

$$\tilde{P} = \begin{pmatrix} -\Delta + V & 0 \\ 0 & -\Delta + V \end{pmatrix}.$$

Note that the functionals type of (7) often met in the solution for example inverse spectral problems with respect to domain. Investigation of these fuctionals makes possible also to study the behavior of the eigenvalues relatively external influences that regularly arise in many applied problems.

The existence of the optimal domains in such problems is investigated in many works and various conditions are derived under with the considered problems are well formulated [1], [11].

The following theorem proved in [9] will be used.

Theorem 1. The functional $\eta_k(D)$ is differentiable in Gatoux sense on K in the direction D_0 and the following formula is valid for its first variation

$$\delta\eta_k(D) = -\max_{\varphi_k^0} \int_{S_{\bar{D}}} \left|\nabla\varphi_k^0(x)\right|^2 \times [P_{\bar{D}}(x) - P_D(x)]\,ds .$$

Here

$$D,\ D_0 \in \Omega, \quad \varphi_k^0(x) = \begin{pmatrix} \varphi_{1k}^0 \\ \varphi_{2k}^0 \end{pmatrix};$$

φ_{1k}^0 , φ_{2k}^0 are k-th eigenfuctions of the problems (7), (8) in the domain D_0 , correspondingly; $|\nabla\varphi(x)|^2 = \sum_{i=1}^{2}\left(\frac{\partial\varphi(x)}{\partial x_i}\right)^2$; s - a boundary element; max is taken over all eigenfactions in the case when the η_k eis a multiple eigenvalue.

Using the theorem we can calculate the variation of the functional $J(D)$

$$\delta J(D) = \delta\lambda_1(D) + \delta\int_D f(x)dx = \delta\eta_k(D) =$$

$$= -\int_{S_D} |\nabla\varphi_1(x)|^2 \times [P_{\bar{D}}(x) - P_D(x)]\, ds + \int_{S_D} f(x)[P_{\bar{D}}(x) - P_D(x)]\, ds =$$

$$= \int_{S_D} \left| f(x) - (\nabla\varphi_1(x)^2 \right| \times [P_{\bar{D}}(x) - P_D(x)]\, ds$$

On this base of this formula it is not difficult to prove the following optimality condition

$$\int_{S_{D^*}} \left[f(x) - |\nabla\varphi_1|^2 \right] \left[P_D(u(x) - P_{D^*}(n(x)) \right] dx \geq 0, \quad \forall D \in K .$$

Now we offer an algorithm for the numerical solution of the considered problem (3) subject to (4), (5).

Algorithm.

Step 1. Chose the initial domain $D_0 \in K$ and assume that $D_i \in K, \quad i = 1,2,...$ are already known.

Step 2. Solve the problem (9) in D_i and find eigenfunction $\varphi_i(x)$.

Step 3. Solve the variational problem

$$\Lambda_i \to \max ,$$

where

$$\Lambda_i = \int_{S_{D_i}} \left| f(x) - (\nabla\varphi_1^{(i)})^2 \right| P(n(x))ds$$

and find convex positively-homogeneous function $\overline{P_i}(x)$.

Step 4. Find the auxiliary domain $\overline{D}_m$ as a subdifferential of the function $\overline{P_i}(x)$ in the point 0.

Step 5. Find the next domain from the relation

$$D_{i+1} = (1-\alpha_i)D_i + \alpha_i \overline{D}_i \text{, where } 0 < \alpha_i < 1 .$$

Step 6. Check up the exactness criteria. If it is not satisfied take $D_i = D_{i+1}$ and go to Step 2. Otherwise stop the iteration.

Using the offered algorithm a computer simulation is carried out for the numerical solution of various shape optimization problems for the eigenvalues of different differential equations describing corresponding mechanical or physical systems [6], [8] (see [10]).

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