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LETTER TO THE EDITOR

Schrödinger operators in spaces of multifunctions defined in multiply-connected domains

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Abstract. Certain problems of quantum physics (for example, the Aharonov–Bohm effect) lead to the eigenvalue problem for a Schrödinger operator with wave multifunctions. For a multiply-connected configuration space with a simplest topology (for example, for a n-dimensional torus) this problem was considered by several authors. In the present paper, by using rigorous mathematical methods we investigate this problem on an arbitrary multi-dimensional smooth manifold (possibly, with a boundary). We carefully define the concept of multifunctions, then we introduce spaces of these objects similar to L_2 and H_0^1. Finally, we present a spectral theorem on the existence of a self-adjoint extension of a Schrödinger operator in the introduced spaces which implies the completeness of the system of eigenfunctions of this operator in the considered functional spaces.

1. Introduction

Certain problems of quantum physics require the study of a Schrödinger equation in spaces of multifunctions. For example, this occurs in the known Aharonov–Bohm effect [1]. In this case, it is known that calculations with multifunctions and without the potential of the magnetic field, and calculations with usual (one-valued) wavefunctions and with the magnetic potential, give identical results. In view of this, it seems natural to consider wave multifunctions in certain cases. Earlier, working in this direction (using the multifunction approach) only configuration spaces with the simplest topology were considered (for example, the problem has been treated when the configuration space is a torus, see [2]).

We consider the general case of an arbitrary connected smooth (of the class C^∞) oriented Riemannian manifold M, $\dim M = d$, with a smooth boundary ∂M which may be empty. We carefully define multifunctions on M by analogy with the simple cases above, introduce spaces similar to L_2 or H_0^1 of these objects and prove the existence of a self-adjoint extension of a Schrödinger operator in these spaces. An approach to the definition of multifunctions, similar to our approach but without mathematical accuracy, is contained in the monograph [3]. Finally, we do not touch upon delicate questions of the Floquet theory (see [2]).

2. Multifunctions

Let C be the set of continuous piecewise smooth maps from $[0, 1]$ into M; $x_0 \in M$ be a fixed point; C_0 be the subset of the set C, $C_0 = \{\gamma \in C | \gamma(0) = x_0\}$; $C_1 = \{\gamma \in C_0 | \gamma(1) = x_0\}$.

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For any two paths $\gamma_1, \gamma_2 \in C$ satisfying $\gamma_1(0) = \gamma_2(1)$ we introduce their product $\gamma_1 \circ \gamma_2 = \gamma$ where $\gamma(t) = \gamma_2(2t)$ if $t \in [0, \frac{1}{2}]$ and $\gamma(t) = \gamma_1(2t-1)$ for $t \in [\frac{1}{2}, 1]$. By analogy, $\gamma^{-1}(t) = \gamma(1-t)$. As usual, we call two paths γ_1 and γ_2 from C_1 equivalent if there exists a continuous homotopy $\sigma(s,t)$, where $s, t \in [0,1]$, such that $\sigma(0,t) = \gamma_1(t)$, $\sigma(1,t) = \gamma_2(t)$ and $\sigma(s,0) = \sigma(s,1) = x_0$. We denote the set of equivalence classes of paths by K. Then, in the set K one has a natural operator of multiplication: if $k_1, k_2 \in K$ and $\gamma_1 \in k_1$, $\gamma_2 \in k_2$, then $k_1 \circ k_2$ is the class $k \in K$ containing the path $\gamma_1 \circ \gamma_2$.

Since M is a Riemannian manifold, M is a metric space with a distance $d(x, y)$ $(x, y \in M)$. Then, one can introduce a distance in the set C, making it a metric space, by the rule

$$\rho(\gamma_1, \gamma_2) = \max_{t\in[0,1]} \min_{s\in[0,1]} d(\gamma_1(t), \gamma_2(s)) + \max_{t\in[0,1]} \min_{s\in[0,1]} d(\gamma_1(s), \gamma_2(t)).$$

(Axioms of the metric space can easily be verified.) Further, by standard arguments, for any $\gamma_0 \in C_1$ there exists $\epsilon > 0$ such that if $\rho(\gamma_0, \gamma) < \epsilon$ for a path $\gamma \in C_1$, then γ is equivalent to γ_0.

Definition 1. We say that a real function θ defined on C_0 is admissible iff

(i) $\theta(\gamma) = 0$ for any path $\gamma \in C_1$ equivalent to the trivial one $\gamma_0(t) \equiv x_0$;

(ii) $\theta(\gamma_1 \circ \gamma_2) = \theta(\gamma_1) + \theta(\gamma_2)$ for any $\gamma_1, \gamma_2 \in C_1$.

Remark 1. One can easily verify that there exists a non-trivial admissible function. Indeed, taking a closed smooth differential 1-form $\omega = \sum_{i=1}^{d} f_i(x)\, \mathrm{d}x_i$ (so that $\mathrm{d}\omega = 0$) and setting for any $\gamma \in C_0$

$$\theta(\gamma) = \int_\gamma \omega$$

we obtain a function θ satisfying definition 1.

Definition 2. We call a complex function f defined on C_0 the multifunction defined on M iff for any $x \in M$ and any $\gamma_1, \gamma_2 \in C_0$ such that $\gamma_1(1) = \gamma_2(1) = x$ one has

$$f(\gamma_2) = f(\gamma_1)\mathrm{e}^{\mathrm{i}\theta(\gamma_1^{-1}\circ\gamma_2)}.$$

Let us show that there exist non-trivial multifunctions. Let $U \subset M \setminus \partial M$ be an open card diffeomorphic to the unit ball $B = B_1(0) = \{z \in R^d \| z| < 1\}$ and f_0 be a complex function defined on M with a support in U. For any $\gamma \in C_0, \gamma(1) \notin U$ we set $f(\gamma) = 0$. Take arbitrary $x_1 \in U$ and fix a path $\gamma_0 \in C_0 : \gamma_0(1) = x_1$. Let $\gamma \in C_0$ be an arbitrary path joining x_0 with $x \in U$. We set

$$f(\gamma) = f_0(\gamma(1))\mathrm{e}^{\mathrm{i}\theta(\gamma_0^{-1}\circ\sigma^{-1}\circ\gamma)}$$

where σ is an arbitrary path from C joining x_1 with $\gamma(1)$ and contained in U. One can easily verify that $f(\gamma)$ is a well-defined multifunction.

Operations of addition of multifunctions and multiplication of a multifunction by a usual (one-valued) function have been introduced naturally ($f(\gamma) = f_1(\gamma) + f_2(\gamma)$ and $g(\gamma) = \alpha(\gamma(1))f(\gamma)$ where f, f_1, f_2 and g are multifunctions and α is a one-valued function). Further, the complex adjoint function to a multifunction f is defined pointwise, too, and it is clear that this is a multifunction with respect to the admissible function $\theta_1 = -\theta$.

3. Continuity and differentiability of multifunctions

Let $\gamma_0 \in C_1$. Since there exists $\epsilon > 0$ such that $\gamma \in C_1$ is equivalent to γ_0 if

$$\rho(\gamma_0, \gamma) < \epsilon \tag{1}$$

a multifunction f as a function of γ satisfying (1) is the usual (one-valued) function of $x = \gamma(1) \in M$, i.e. locally any multifunction is a function of points of the manifold M. (Indeed, if γ_1 and γ_2 are paths from C_0 satisfying (1) and $\gamma_1(1) = \gamma_2(1)$, then these two paths are homotopic, hence $f(\gamma_1) = f(\gamma_2)$ and therefore f is a function ϕ only of $x = \gamma_i(1)$.) Using these arguments, we introduce the following.

Definition 3. A multifunction f is called continuous in a point γ_0 (resp., infinitely differentiable in $M \setminus \partial M$) if there exists $\epsilon > 0$ such that the corresponding function ϕ is continuous in x in a neighbourhood of the point $\gamma_0(1)$ (resp., each function ϕ is infinitely differentiable in a neighbourhood of the point $x_0 = \gamma_0(1) \notin \partial M$).

Definition 4. Let S be the set of all $x \in M$ such that for a given continuous multifunction f there exists a path $\gamma, \gamma(1) = x$, such that $f(\gamma) \neq 0$ and let $\bar{S}$ be the closure of the set S. We call $\bar{S}$ the support of f ($\bar{S} = \text{supp}(f)$).

Definition 5. By D_0^∞ we denote the set of infinitely differentiable in $M \setminus \partial M$ multifunctions, the support of each satisfying

$$\text{dist}(\bar{S}, \partial M) > 0$$

where $\text{dist}(A, B) = \inf_{x \in A, y \in B} d(x, y)$.

4. The space of square-integrable multifunctions

Take arbitrary multifunctions f and g. We set $(f\bar{g})(\gamma) = f(\gamma)\bar{g}(\gamma)$ where $\bar{g}$ is the complex adjoint multifunction to g. We state that $f\bar{g}$ is a usual (one-valued) function on M depending only on $x = \gamma(1)$. Let us prove this statement.

Take arbitrary $\gamma_1, \gamma_2 \in C_0$ such that $\gamma_1(1) = \gamma_2(1) = x \in M$. We should prove that $f(\gamma_1)\bar{g}(\gamma_1) = f(\gamma_2)\bar{g}(\gamma_2)$, only, but according to the above results (see section 2) $f(\gamma_1) = e^{i\theta} f(\gamma_2)$ and $\bar{g}(\gamma_1) = e^{-i\theta}\bar{g}(\gamma_2)$ for some θ, and thus the statement is proved.

One can verify that the expression $\|f\| = \{\int_M f\bar{f}\}^{\frac{1}{2}}$ is a norm in the space D_0^∞. Using this fact, we introduce the following.

Definition 6. We denote by F_2 the completion of the space D_0^∞ with the norm $\|.\|$. In fact, F_2 is a Hilbert space and D_0^∞ is a dense linear subspace in this space. By $(.,.)$ we denote the scalar product in the space F_2 ($(f, g) = \int_M (f\bar{g})(x)$).

5. Laplacian

Let U be an open card on M with a coordinate function $\phi : B \to U$ where B is a d-dimensional open ball from R^d so that $\phi(z) = x \in M$ and $z = (z_1, ..., z_d) \in B$. For smooth in U usual (one-valued) functions f the known Laplace–Beltrami operator takes the following form:

$$\Delta f = \sum_{i,j=1}^{d} (\det(g_{i,j}(z)))^{-\frac{1}{2}} \frac{\partial}{\partial z_i} \left[((\det(g_{i,j}(z)))^{\frac{1}{2}} g^{i,j}(z) \frac{\partial}{\partial z_j} f(\phi(z)) \right]$$

where $g_{i,j}(z)$ and $g^{i,j}(z)$ are, respectively, covariant and contravariant components of the Riemannian tensor. It is essential to note that if M is a domain in an Euclidian space with the corresponding metric then the Laplace–Beltrami operator becomes the usual Laplacian. Therefore, it is natural to give the following.

Definition 7. Let $f \in D_0^\infty$, let U be the above open card on M and $\gamma_0 \in C_0$ be a path such that $\gamma_0(1) = x_0 \in U$. Then, since locally f is a function $\psi(x)$ of points $x \in M$ from a neighbourhood of the point x_0, we set

$$\Delta f(\gamma) = \Delta\psi(x)$$

for all paths γ sufficiently close to γ_0. We call the operator Δ the Laplacian or the Laplace–Beltrami operator. One can easily verify that $\Delta f(\gamma)$ is a multifunction in the sense of definition 2 with the same admissible function θ.

Lemma 1. The operator $-\Delta$ is symmetric and non-negative in the space D_0^∞ equipped by the scalar product from F_2.

Proof. As above, for any $\phi, \psi \in D_0^\infty$ $\phi(x)\bar{\psi}(x)$ is a usual (one-valued) function on M. Let $R = \mathrm{supp}(\phi) \bigcup \mathrm{supp}(\psi)$. Then, R is a compact set and $\mathrm{dist}(R; \partial M) > 0$. Let $U_1, \ldots, U_l$ be its covering by open in M cards diffeomorphic to B and let $\sigma_1, \ldots, \sigma_l$ be smooth (σ_k are infinitely differentiable) non-negative functions defined on M such that $\mathrm{supp}(\sigma_k) \subset U_k$, $k = \overline{1, l}$ and $\sum_{k=1}^{l} \sigma_k(x) = 1$ for all $x \in R$. Then, one obtains (because the Laplacian is symmetric on usual functions)

$$\begin{aligned}(\Delta\phi, \psi) &= \sum_{k,m=1}^{l} (\Delta\phi_k, \psi_m) = \sum_{k,m=1}^{l} (\Delta\tilde{\phi}_k, \tilde{\psi}_m) = \sum_{k,m=1}^{l} (\tilde{\phi}_k, \Delta\tilde{\psi}_m) \\ &= \sum_{k,m=1}^{l} (\phi_k, \Delta\psi_m) = (\phi, \Delta\psi)\end{aligned}$$

where $\tilde{\phi}_k$ and $\tilde{\psi}_m$ are usual (one-valued) functions with supports in U_k and $U_k \bigcap U_m$, respectively, which are obtained by fixing any $\gamma_k \in C_0$ ($k = \overline{1, l}$) such that $\gamma_k(1) \in U_k$ and taking $\tilde{\phi}_k(x) = \phi_k(\eta_k \circ \gamma_k)$, $\tilde{\psi}_m(x) = \psi_m(\eta_k \circ \gamma_k)$ for $x = \eta_k(1)$ where $\eta_k(0) = \gamma_k(1)$, $\eta_k(t) \in U_k \bigcap U_m$ and $\eta_k \in C$. By analogy, we introduce functions $\tilde{\phi}$: $\tilde{\phi}(x) = \phi(\eta_k \circ \gamma_k)$ for $x = \eta_k(1) \in U_k$. Thus, the Laplacian is symmetric.

By analogy,

$$\begin{aligned}(-\Delta\phi, \phi) &= \sum_{k,m=1}^{l} (-\Delta\phi_k, \phi_m) = \sum_{k,m=1}^{l} \int_{G_{k,m}} \sum_{i,j=1}^{d} (\det(g_{i,j}))^{\frac{1}{2}} g^{i,j}(z) \frac{\partial}{\partial z_i}\tilde{\phi}_k(z) \overline{\frac{\partial}{\partial z_j}\tilde{\phi}_m(z)} \\ &= \sum_{k,m=1}^{l} \int_{G_{k,m}} \sigma_k(z)\sigma_m(z) \sum_{i,j=1}^{d} (\det(g_{i,j}))^{\frac{1}{2}} g^{i,j}(z) \frac{\partial}{\partial z_i}\tilde{\phi}(z) \overline{\frac{\partial}{\partial z_j}\tilde{\phi}(z)} + J \qquad (2)\end{aligned}$$

where $G_{k,m}$ is the pre-image of $U_k \bigcap U_m$ and we mean that the integrand is non-zero only in $U_k \bigcap U_m$. Now, to prove lemma 1, it suffices to prove that $J = 0$. Not writing the whole expression for J (one can easily do it), we prove that

$$\int_{G_{k,m}} \sum_{k,m=1}^{l} \sum_{i,j=1}^{d} \left[\frac{\partial}{\partial z_i}\sigma_k(z)\right] \sigma_m(z) (\det(g_{i,j}(z)))^{\frac{1}{2}} g^{i,j}(z) \left(\tilde{\phi}\overline{\frac{\partial}{\partial z_j}\tilde{\phi}}\right)(z)\, \mathrm{d}z = 0. \qquad (3)$$

Then, by analogy, one can repeat this proof for all other terms in the expression for J showing the equality $J = 0$.

To prove (3), we observe that the expression $(\tilde{\phi}\overline{\frac{\partial}{\partial z_j}\tilde{\phi}})(z)$ generates a usual (one-valued) smooth vector field on M. Therefore, at any point z the expression

$$\frac{\partial}{\partial z_i}\sigma_k(z)g^{i,j}(z)\tilde{\phi}(z)\overline{\frac{\partial}{\partial z_j}\tilde{\phi}(z)}$$

is a scalar product of two vectors. Hence,

$$\sum_{k=1}^{l}\frac{\partial}{\partial z_i}[\sigma_k(z)]g^{i,j}(z)\tilde{\phi}(z)\overline{\frac{\partial}{\partial z_j}\tilde{\phi}(z)} = \frac{\partial}{\partial z_i}\left[\sum_{k=1}^{l}\sigma_k(z)\right]g^{i,j}(z)\tilde{\phi}(z)\overline{\frac{\partial}{\partial z_j}\tilde{\phi}(z)} = 0$$

and, thus, lemma 1 is proved.

6. Spectral theory

Let $V(x) \geqslant -V_0$ be a real continuous function on M where $V_0 =$ const. independent of $x \in M$. Consider the operator $H = -\Delta + V(x)$. By the above arguments, this is a bounded from below symmetric operator on D_0^∞. Therefore, it has a self-adjoint extension in F_2 with the same lower boundary.

If the manifold M is compact, we can present a more complete information about the operator H. In fact, in this case H has a self- adjoint extension with a discrete spectrum, only, which consists of eigenvalues $\lambda_n > 0$ $(n = 1, 2, 3, \ldots)$ monotonously converging to $+\infty$, and to any λ_n there corresponds a finite number of orthonormal eigenfunctions; two eigenfunctions corresponding to non-equal eigenvalues λ_n and λ_m are orthogonal in F_2. To prove this statement, it suffices to prove that there exists $a > 0$ such that the operator $(H + aI)^{-1}$ is compact, positive and symmetric (here I is the identical operator).

Let $H_1 = H_1(M)$ be the completion of the space D_0^∞ with the norm $\|f\|_1 = ((H + aI)f, f)^{\frac{1}{2}}$ where $a = V_0 + 1$.

Lemma 2. Let M be a compact manifold. Then, the space H_1 is compactly embedded in F_2.

Proof. First, since $\|f\|_1 \geqslant \|f\|$ for all $f \in D_0^\infty$, the space H_1 is continuously embedded into F_2 for the manifold M without the requirement of its compactness. Let M be a compact manifold. Fix an arbitrary finite covering $U_1, \ldots, U_l$ of M by open cards each of which is diffeomorphic to the ball B or the half-ball $B_1 = \{z \in B|\ z_1 \geqslant 0\}$. Let $\sigma_1, \ldots, \sigma_l$ be the corresponding smooth partition of unity (so that $\sum_{i=1}^{l}\sigma_i(x) = 1$ for all $x \in M$, $\sigma_i(x) \geqslant 0$ and $\mathrm{supp}(\sigma_i) \subset U_i$). Further, we take arbitrary paths $\gamma_i \in C_0$ leading to some $x_i \in U_i$. As in the proof of lemma 1, let $f_k(x)$ $(x \in M)$ be (one-valued) functions in U_k obtained by taking paths $\beta_k \subset U_k$, $\beta_k(0) = x_k$, $\beta_k(1) = x$ and setting $f_k(x) = f(\beta_k \circ \gamma_k)$. Then, according to formula (2) (where $J = 0$), one has for $f \in D_0^\infty$, $\|f\|_1$ greater or equal to

$$\left\{\sum_{k,m=1}^{l}\int_{G_{k,m}}\sigma_k(z)\sigma_m(z)\det(g_{i,j}(z))^{\frac{1}{2}}\left[\sum_{i,j=1}^{d}g^{i,j}(z)\frac{\partial}{\partial z_i}f_k(z)\overline{\frac{\partial}{\partial z_j}f_k(z)} + f_k\bar{f}_k\right]\mathrm{d}z\right\}^{\frac{1}{2}}.$$

Obviously, there exists $r > 0$ such that the pre-images $E_{k,m}$ of the domains

$$V_{k,m} = \{x \in U_k \bigcap U_m | \sigma_k(x) > r, \sigma_m(x) > r\}$$

cover M. Therefore, $\|f\|_1 \geqslant C\|f_k(z)\|_{H^1(E_{k,m})}$ for all k, m. Hence, if R is a set of functions bounded in the norm of H_1, then for all $k, m = \overline{1, l}$ the sets $R_{k,m}$ of corresponding functions $f_k(z)$ are compact in $L_2(E_{k,m})$. This easily implies the statement of lemma 2.

Consider the equation

$$(H + aI)u = f \in F_2 \tag{4}$$

with the unknown function $u \in H_1$. Multiplying(4) by $v \in H_1$, we find

$$(u, v)_1 = (f, v) \tag{5}$$

for all $v \in H_1$. In view of the equality (5), for any $f \in F_2$ there corresponds a unique $u \in H_1$ such that the equality (5) takes place for all $v \in H_1$, and, in addition,

$$\|u\|_1 \leqslant C\|f\| \tag{6}$$

(for proofs, see [4]; they are based on the usual technique of proving the existence and uniqueness of a generalized solution to a linear elliptic equation).

By B we denote the operator mapping arbitrary $f \in F_2$ into $u \in H_1$ where u satisfies (5). According to (6) and lemma 2, B is a compact operator in F_2.

Further, since for $u, v \in H_1$ one has

$$(Bu, v)_1 = (u, v) = \overline{(v, u)} = \overline{(Bv, u)_1} = (u, Bv)_1 \tag{7}$$

the operator B is self-adjoint in H_1. By analogy, B is a non-negative operator in H_1.

To prove that B is a compact operator in H_1, consider an arbitrary bounded set $R \subset H_1$. In particular, any sequence $\{f_n\} \subset R$ contains a subsequence $\{f_{n_k}\}$ strongly converging in F_2. Therefore, the sequence Bf_{n_k} strongly converges in H_1, and the compactness of the operator B in H_1 is proved.

According to the Hilbert–Schmidt theorem, there exists an orthonormal basis in H_1 consisting of eigenfunctions of the operator B with corresponding eigenvalues $\lambda_n \geqslant 0$ of finite multiplicities and there exists a monotonous limit $\lim_{n\to\infty} \lambda_n = 0$. We denote the corresponding eigenfunctions of the operator B by u_n accepting that each eigenvalue λ_n appears in the sequence $\{\lambda_n\}$ so many times which is its multiplicity.

Then, obviously the space F_2 is an analogue of the space L_2, and, since we consider applications of our construction in quantum mechanics, we need to prove a spectral expansion for the operator H in F_2. However, this result follows from the above one. Indeed, since $u_n \in F_2$ for all n and since the space H_1 is dense in F_2, one has that $\{u_n\}$ is a basis in F_2 which is orthogonal by the equality (7). Finally, if $Bu = 0$ for $u \in F_2$, then according to (7) one has $(u, v) = 0$ for all $v \in H_1$, hence $u = 0$. Thus, there exists an operator B^{-1} mapping the image of the operator B into F_2. Further, since for $u \in D_0^\infty$ $B^{-1}u = (H + aI)u$ (i.e. if $u \in D_0^\infty$, $B^{-1}u$ is determined and coincides with $(H + aI)u$), the operator B^{-1} is self-adjoint in F_2 and it is a self-adjoint extension of the operator $(H + aI)$. Thus, we have proved the following result:

Theorem 1. Let the manifold M be compact. Then, the operator H with the domain D_0^∞ considered in F_2 has a self-adjoint extension with only a discrete spectrum $\{\lambda_n^{-1}\}$ (here $\lim_{n\to\infty} \lambda_n^{-1} = +\infty$) where each eigenvalue λ_n^{-1} is of a finite multiplicity.

A brief variant of the paper (without proofs) will be published in [5].

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