Self-Adjoint Extension Operator Theory Applied to the Confinement of Quantum Systems

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Abstract: *In this talk, we discuss several applications of self-adjoint extension theory to the confinement of quantum systems, with particular emphasis on the Aharonov–Bohm effect. In quantum mechanics, the choice of a Hilbert space and a self-adjoint Hamiltonian — also known as the Schrödinger operator — is essential for ensuring the well-posedness of a quantum system, that is, the existence and uniqueness of solutions to Schrödinger's equation. Typically, for a particle confined to an open set* Ω*, the Hilbert space is* $L^2(\Omega)$*, and the Hamiltonian is obtained through a quantization procedure. Different self-adjoint extensions of this operator correspond to distinct, well-posed quantum systems. When* Ω *does not coincide with the whole space, as in the Aharonov–Bohm setting, the operator generally admits infinitely many self-adjoint extensions, and appropriate boundary conditions must be specified. Moreover, recent developments in the so-called dynamical confinement — where an initial state supported in* Ω *remains in* Ω *throughout the time evolution — have shown that the well-posedness of the model is, in a certain sense, tied to the commutation of the global Hamiltonian with the orthogonal projection onto* Ω*. In this talk, we present three approaches for constructing self-adjoint Hamiltonians — the self-adjoint extension method, the confinement method and the dynamical confinement method — and illustrate their application to the Aharonov–Bohm effect.*

Keywords: *Quantum Mechanics, Aharonov-Bohm effect, Quantum confinement*

1 Introduction

Non-relativistic quantum mechanics is based on a number of axioms that establish the fundamental mathematical structure of the theory (see [7, 16] for general references on the subject). These axioms ensure the well-posedness of the quantum problem, that is, the existence and uniqueness of solutions to the evolution equations. In this framework, states of a quantum system are normalized elements of a separable Hilbert space $\mathcal{H}$ — called wave functions — and the observables are self-adjoint operators A with dense domain $\mathrm{dom}(A) \subset \mathcal{H}$. The evolution of a quantum system is governed by Schrödinger's equation,

$$i\hbar \frac{d}{dt}\psi(x,t) = H\psi(x,t), \tag{1}$$

with initial condition $\psi(x,0) = \psi_0(x)$, where H, the energy observable defined on $\mathcal{H}$, is called the Hamiltonian. Stone's Theorem then ensures that Equation (1) has a unique solution for all $\psi_0 \in \mathrm{dom}(H)$ and all t if, and only if, the Hamiltonian H is self-adjoint. The solution is given by the one-parameter strongly continuous unitary group $\psi(t) = e^{-itH}\psi_0$, whose generator is H. Thus, for a quantum system to be mathematically well defined, one must specify a Hilbert space $\mathcal{H}$ and a self-adjoint Hamiltonian.

Regarding the Hilbert space, the usual interpretation of a state ψ is probabilistic. More precisely, ψ is a complex-valued function $\psi : \Omega \to \mathbb{C}$ such that

$$\rho_t(S) = \int_S |\psi(x,t)|^2 \, dx \tag{2}$$

represents the probability of finding the particle in the region S at time t. In particular, $\int_\Omega |\psi(x,t)|^2 \, dx = 1$ for all t, and therefore $\psi(\cdot, t) \in L^2(\Omega)$. For this reason, $L^2(\Omega)$ is the natural Hilbert space for a quantum particle confined to the open region Ω, according to the standard interpretation of the wave function.

For the Hamiltonian H, the construction of the energy operator is a central problem related to the quantization of systems with boundaries. Its action on smooth functions with compact support $C_0^\infty(\Omega)$ — called the initial Hamiltonian (not self-adjoint in general) — is typically given by

$$\begin{cases} \dot{H} = -(\nabla - i\mathbf{A})^2 + V, \\ \operatorname{dom}(\dot{H}) = C_0^\infty(\Omega), \end{cases} \tag{3}$$

for mass $m = 1/2$ and Planck's constant $\hbar = 1$, where $\mathbf{A}$ is the magnetic potential and V the electric potential on Ω. This expression is obtained from the classical Lagrangian by replacing the classical momentum $\mathbf{p}$ with the quantum momentum operator $-i\nabla$. For $\dot{H}$ to define a self-adjoint operator, one must specify a domain $\operatorname{dom}(H)$ such that H is a self-adjoint extension of $\dot{H}$.

If $\Omega = \mathbb{R}^3$, then $\dot{H}$ is essentially self-adjoint and has a unique self-adjoint extension, given by its closure $H = \overline{\dot{H}}$. In this case, the maximal domain

$$\operatorname{dom}(H) = \{\psi \in L^2(\mathbb{R}^3) : H\psi \in L^2(\mathbb{R}^3)\}$$

is the natural choice for defining the self-adjoint Hamiltonian, where derivatives are taken in the weak sense. However, if $\Omega \neq \mathbb{R}^3$, there is no canonical domain guaranteeing self-adjointness, since the initial operator $\dot{H}$ admits infinitely many self-adjoint extensions. This situation is precisely what occurs in the Aharonov–Bohm effect.

2 The Aharonov–Bohm effect

Consider an infinite cylindrical solenoid with radius $a > 0$ carrying a constant current. The magnetic field is then confined to the interior of the solenoid, while a vector potential $\mathbf{A}$ defined by

$$\mathbf{A}(x,y) = \frac{\kappa}{|x|^2}(-y, x) \tag{4}$$

is present in the exterior region $\Omega = \{x \in \mathbb{R}^2 : \|x\| > a\}$. Note that $\nabla \times \mathbf{A} = \mathbf{B} = 0$ and $\nabla \cdot \mathbf{A} = 0$ in Ω. If a charged particle is confined to Ω, then the associated Hilbert space is $L^2(\Omega)$, and the initial Hamiltonian is

$$\begin{cases} \dot{H} = -(\nabla - i\mathbf{A})^2, \\ \operatorname{dom}(\dot{H}) = C_0^\infty(\Omega). \end{cases} \tag{5}$$

Observe that the particle is subject to a magnetic potential $\mathbf{A} \neq 0$ but not to a magnetic field, since $\mathbf{B} = 0$ in Ω. The Aharonov–Bohm effect [2] states that the particle can nevertheless be influenced by the magnetic flux generated by $\mathbf{A}$, even without coming into contact with the magnetic field confined inside the solenoid. After experimental confirmation [17], attention turned to the mathematical modelling of the effect. For instance, in [15] the author analyzes the scattering of electrons by a cylinder containing a current-carrying solenoid, relating the scattering cross sections to the magnetic flux. A similar analysis appears in [3], but for more general obstacles in the high-velocity limit. In [8], the author proves that the first eigenvalue, or ground-state energy, depends on the magnetic flux, even for non-circular solenoids in $\mathbb{R}^2$. In [1], the authors classify all self-adjoint extensions using von Neumann's theory and related methods. For non-smooth solenoids, a classification of all admissible boundary conditions is given in [13].

3 Confinement by boundary conditions

There are several ways to relate boundary conditions to self-adjoint extensions. By von Neumann's theory, each self-adjoint extension of a Hermitian operator T is in one-to-one correspondence with a unitary transformation between its deficiency subspaces. More precisely, consider the deficiency subspaces

$$K_{\pm}(T) = \mathrm{Ker}(T^* \pm i\mathbf{1})$$

associated with T. Then, with respect to the graph inner product of T^*, we have

$$\mathrm{dom}(T^*) = \mathrm{dom}\,\overline{T} \oplus K_+(T) \oplus K_-(T), \tag{6}$$

and if the deficiency subspaces have equal dimensions, $n_- = n_+$, the operator T admits self-adjoint extensions T_U parametrized by all unitary operators

$$U : K_-(T) \to K_+(T).$$

In [1], the authors determine all self-adjoint extensions of the operator $\dot{H}$ on the punctured plane using von Neumann's theory, showing that they are naturally associated with boundary conditions at the origin and analyzing the scattering and spectral properties of each self-adjoint extension.

Another technique is based on boundary triples. One begins with the boundary form of a Hermitian operator T, that is, the sesquilinear form

$$\Gamma : \mathrm{dom}\,T^* \times \mathrm{dom}\,T^* \to \mathbb{C}$$

defined by

$$\Gamma(\xi, \eta) := \langle T^*\xi, \eta\rangle - \langle \xi, T^*\eta\rangle. \tag{7}$$

A triple $(\mathbf{h}, \rho_1, \rho_2)$ consisting of a Hilbert space $\mathbf{h}$ and linear maps $\rho_i : \mathrm{dom}(T^*) \to \mathbf{h}$ with dense range is called a boundary triple for T if

$$a\,\Gamma(\xi, \eta) = \langle \rho_1(\xi), \rho_1(\eta)\rangle - \langle \rho_2(\xi), \rho_2(\eta)\rangle, \quad \forall\, \xi, \eta \in \mathrm{dom}(T^*), \tag{8}$$

for some nonzero $a \in \mathbb{C}$. Under these conditions, if T has equal deficiency indices, the self-adjoint extensions T_U are given by

$$\mathrm{dom}\,T_U := \{\xi \in \mathrm{dom}(T^*) : \rho_2(\xi) = U\rho_1(\xi)\}, \qquad T_U\xi = T^*\xi, \tag{9}$$

where $U : \mathbf{h} \to \mathbf{h}$ is any unitary operator. In [10], the authors obtain and study self-adjoint extensions of the operator $\dot{H}$ for a solenoid of nonzero radius. In [13], the authors find all self-adjoint extensions corresponding to the non-smooth solenoid boundary.

4 Confinement by potential barriers

Another way to ensure the well-posedness of the problem is to add a confining potential so that the initial Hamiltonian becomes essentially self-adjoint. For instance, in [9, 4], the authors proved that by adding a sufficiently singular magnetic or electric potential, the initial operator has a unique self-adjoint extension. Hence, no boundary conditions are needed and the dynamics are well defined using only the initial operator. In [11], we proved the following result:

Theorem 1. *Let V be any smooth scalar potential on Ω such that there exists $\varepsilon_V > 0$ for which, setting $d(x) := \inf_{y\in\partial\Omega} \|x - y\|$, we have*

$$V(x) \geq \frac{1}{d(x)^2}, \qquad \forall x \in \Omega, \quad d(x) < \varepsilon_V. \tag{10}$$

Then the operator

$$\dot{H} = -(\nabla - i\mathbf{A})^2 + V, \qquad \mathrm{dom}(\dot{H}) = C_0^\infty(\Omega), \tag{11}$$

is essentially self-adjoint.

In this situation, the well-posedness of the problem does not arise from the choice of a boundary condition, but rather from the repulsive barrier generated by V. This leads to an interesting situation described in [12], where we proved the following:

Theorem 2. *Consider $\Omega = \mathbb{R}^2 \setminus \{0\}$, the radial scalar potential $V(r) = \alpha/r^2$ with $\alpha < 1$, and the Aharonov–Bohm initial Hamiltonian* (11). *Then the deficiency indices of the operator $\dot{H}$ equal the number of integers $m \in \mathbb{Z}$ satisfying*

$$|m - \kappa| < \sqrt{1-\alpha}. \tag{12}$$

In particular, for fixed $\alpha < 1$, the family of self-adjoint extensions of $\dot{H}$ is parametrized by different matrix sets depending on κ, the magnetic parameter. This offers an alternative viewpoint on the Aharonov–Bohm effect in such cases.

5 Dynamical confinement

All of the above considerations regarding the definition of a Hamiltonian for the confined Aharonov–Bohm operator rely on a *kinematical* approach to the problem, in which a self-adjoint operator is obtained directly by specifying its domain: in the first case by choosing a boundary condition, and in the second by introducing a confining potential. More recently, however, a *dynamical* approach to confinement has been developed. Results concerning self-adjoint extensions of operator restrictions can be applied to obtain a global dynamical formulation of such quantum confined systems [6, 5].

In the dynamical approach, the Hamiltonian H is defined on the whole space $\mathbb{R}^2$, not only on Ω, and the confinement becomes a property of the dynamics: if the initial condition of the Schrödinger equation has support in the expected confining region, then the corresponding solution will remain supported there for all future times. To implement this idea, one starts with a nonconfining Hamiltonian H_0, which represents the natural choice for the unconfined system, and then investigates all possible Hamiltonians H that (i) exhibit the quantum dynamical confinement property and (ii) reproduce the action of H_0 on a suitable subspace; moreover, each such confining operator is self-adjoint on its maximal domain.

More precisely, since

$$L^2(\mathbb{R}^2) = L^2(\Omega_1) \oplus L^2(\Omega_2), \qquad \Omega_1 = \Omega, \quad \Omega_2 = \overline{\Omega}^{\,c},$$

we may define the orthogonal projection Q_Ω onto $L^2(\Omega)$. With this, the following notion was introduced in [6]:

Definition 3. *Let* $\mathrm{H}_0 : \mathrm{dom}\,\mathrm{H}_0 \subset \mathrm{L}^2(\mathbb{R}^d) \to \mathrm{L}^2(\mathbb{R}^d)$ *be a fixed self-adjoint operator. We say that another self-adjoint operator* $\mathrm{H} : \mathrm{dom}\,\mathrm{H} \subset \mathrm{L}^2(\mathbb{R}^d) \to \mathrm{L}^2(\mathbb{R}^d)$ dynamically confines H_0 to Ω *when the following two properties hold:*

(C1) $\mathrm{Q}_\Omega(\mathrm{dom}\,\mathrm{H}) \subset \mathrm{dom}\,\mathrm{H}$ *and the commutator satisfies*

$$[\mathrm{Q}_\Omega, \mathrm{H}]\psi = \mathrm{Q}_\Omega \mathrm{H}\psi - \mathrm{H}\mathrm{Q}_\Omega\psi = 0, \qquad \forall\, \psi \in \mathrm{dom}\,\mathrm{H};$$

(C2) if $\psi \in \operatorname{dom} \mathrm{H}_0$ is an eigenstate of Q_Ω, then $\psi \in \operatorname{dom} \mathrm{H}$ and $\mathrm{H}\psi = \mathrm{H}_0\psi$.

Let $R_i : L^2(\mathbb{R}^2) \to L^2(\Omega_i)$ denote the restriction operator and $E_i : L^2(\Omega_i) \to L^2(\mathbb{R}^2)$ the extension-by-zero operator. Given a self-adjoint operator H_0, define

$$S_j : C_0^\infty(\Omega_j) \subset L^2(\Omega_j) \to L^2(\Omega_j), \qquad S_j\psi = R_j H_0 E_j \psi, \quad j = 1, 2.$$

For the Aharonov–Bohm operator, we proved the following result in [14]:

Theorem 4. *Consider the operator $\dot{H}_0$ defined by (5), which is essentially self-adjoint, and let H_0 be its self-adjoint extension. Then the operator*

$$H = H_1 \oplus H_2,$$

where each H_j is a self-adjoint extension of S_j, dynamically confines H_0 to Ω.

With this result at hand, it becomes possible to study gauge transformations and boundary potentials for the operator H.

6 Conclusion

The Aharonov-Bohm effect is an interesting case of a quantum confined system, since by its nature, the particle must be excluded from the magnetic field and, so, confined to a region Ω different from $\mathbb{R}^d$. The existence of an infinite number of self-adjoint extension for the usual initial Hamiltonian makes the AB effect a rich field of research in mathematical-physics, from self-adjoint extension operator theory, spectral theory and scattering theory.

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