STATEMENT OF INTERESTS

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My research interests are in the edge between analysis and mathematical physics. In particular I am interested in applications of operator theory and functional analysis to problems stemming from quantum mechanics (self-adjointness, spectra of operators, resolvent formulas, . . . ) and in analytical mechanics (dynamics of Hamiltonian systems with a large number of degrees of freedom, Fermi-Pasta-Ulam problem).

1. CURRENT RESEARCH PROJECTS

1.1. Self-adjointness for Quantum Hamiltonians.

Self-adjoint extension theory constitute a well-established branch of functional analysis and operator theory, with deep-rooted motivations and applications, among others, in the boundary value problems for partial differential equations and in the mathematical methods for quantum mechanics.

In quantum mechanics, it is postulated that every observable is represented as a self-adjoint operator on some Hilbert space $H$. In most cases, physical reasoning provides a formal expression for such operators without specifying their domains, an information that is necessary to qualify self-adjointness.

One standard way to assign domains to such operators, especially when they are different operators, is to take their minimal and maximal realisations (see e.g. [32, Section 4.1] or [52, Section 1.3]) which are always densely defined and, in the case of physical interest, are one the adjoint of the other.

In certain circumstances the two above-mentioned operators coincide, which implies that the formal operator has a unique self-adjoint realisation on $H$. But this is not always the case, and given a formal operator $\tilde{A}$, if its minimal realisation $A_{\text{min}}$ and its maximal one $A_{\text{max}}$ are different, any self-adjoint realisation $A_{\text{s.a.}}$ satisfies $A_{\text{min}} \subset A_{\text{s.a.}} \subset A_{\text{max}}$. Each such realisation corresponds to a different physical observable. A major issue in any quantum mechanical model [46, Section VIII.11] is to classify all self-adjoint realisations of the formal operator, hence all physical observables associated with it.

At the highest level of generality, von Neumann theory [55] solves the problem of classifying all self-adjoint realisations of $\tilde{A}$ in terms of unitary operators $U : \ker(A_{\text{max}} - i) \to \ker(A_{\text{max}} + i)$, the condition that such subspaces be isomorphic being necessary and sufficient for the problem to have a solution. In this theory each extension $A_U$ is determined by an explicit and constructive recipe, given $U$ and the above subspaces.

A relevant special case is when $A_{\text{min}}$ is semi-bounded – one customarily assumes it to be bounded from below – which is in fact a typical situation in the quest for stable quantum mechanical Hamiltonians. In this case, $\ker(A_{\text{max}} - i)$ and $\ker(A_{\text{max}} + i)$ are necessarily isomorphic, which guarantees the existence of self-adjoint extensions. The first systematic extension theory for semi-bounded operators is due to Kreǐn [38] and its development is known as the Kreǐn-Višík-Birman extension theory (KVB). It consists of an explicit and extremely convenient classification of all self-adjoint extensions of a given semi-bounded and densely defined

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symmetric operator \( A_{\text{min}} \) both in the operator sense and in the quadratic form sense. In [26], together with A. Michelangeli and A. Ottolini, I revisited the key results of the KVB theory including missing details and additional properties with their own interest. Briefly speaking, KVB theory provides a parametrisation of the self-adjoint extensions of the semi-bounded from below operator \( A_{\text{min}} \) in terms of self-adjoint operators \( B \) acting on Hilbert subspaces of \( \ker(A_{\text{max}} + \lambda) \) where \( \lambda \in \mathbb{R} \) exceeds the absolute value of the bottom of \( A_{\text{min}} \). In many respects, KVB theory turns out to be more informative as compared to von Neumann’s, in particular:

- the parametrisation \( B \leftrightarrow A_B \) identifies special subclasses of extensions of \( A_{\text{min}} \), such as those whose bottom is above a prescribed level, in terms of a corresponding subclass of parameters \( B \);
- the operators \( B_F \) and \( B_N \) labelling the Friedrichs extension \( A_F = A_{B_F} \) and the Krein-von Neumann extension \( A_N = A_{B_N} \) are explicitly known a priori;
- further relevant information concerning each extension, including invertibility, semi-boundedness, special features of its negative spectrum (finiteness, multiplicity, accumulation points) turn out to be controlled by the analogous properties of the extension parameter \( B \);
- for semi-bounded operators, KVB theory provides in addition a classification of the corresponding quadratic forms.

During my doctoral studies a considerable part of my research has been focused on the qualification of self-adjoint realisations for formal Hamiltonians of physical relevance that are not essentially self-adjoint and hence are physically ambiguous. KVB theory turned out to be a very efficient tool. In this context, my works [25, 27, 24] were structured according to the following scheme:

- one common feature of the problems is the presence of a symmetry that allows one to reduce the analysis to ordinary differential operators on the half-line;
- first, reduced operators are analysed by means of Weyl’s limit-point/limit-circle criterion of essential self-adjointness (see [59]);
- the kernel of the of the adjoint of the reduced one-dimensional ordinary differential operator is known explicitly in terms of special functions, specifically confluent hypergeometric, Whittaker and modified Bessel functions;
- the inverse of a distinguished extension can be written explicitly using Green function methods;
- further, one estimates the behaviour close to the origin of functions in the domain of the minimal realisation of the reduced ordinary differential operator;
- at this point all ingredients to apply KVB theory are known explicitly, which allows one to identify the domains of all self-adjoint realisations by suitable boundary conditions at the origin connecting the ‘regular part’ to the ‘singular part’ of every function in the domain of the maximal realisation of the ordinary differential operator.

1.2. Dirac-Coulomb Operators in the critical regime.

The Dirac-Coulomb system is a model for a relativistic electron subjected to the electrostatic attraction of a positively-charged nucleus placed at the origin. The formal expression of the Hamiltonian is

\[
H = -i\mathbf{\alpha} \cdot \nabla + \frac{\nu}{|x|} + \beta
\]

as an operator acting on \( L^2(\mathbb{R}^3, \mathbb{C}^4) \). Here \( \mathbf{\alpha} = (\alpha_1, \alpha_2, \alpha_3) \) and \( \alpha_1, \alpha_2, \alpha_3, \beta \) are \( 4 \times 4 \) hermitian and anticommuting matrices (see e.g. [22, Eq. (5)]) and \( \nu \in \mathbb{R} \) is
the charge of the nucleus. The problem of the self-adjointness of $H$ has a long story that dates back to Rellich [48] and Kato [37] who established its self-adjointness for $|\nu| < \frac{1}{2}$ by means of perturbative arguments. Adapting the perturbative argument several authors proved the essential self-adjointness of the operator reaching the optimal value of $\nu = \sqrt{\frac{3}{2}}$ [47, 33, 51, 14, 17, 39, 58].

Many subsequent works [50, 40, 60, 16, 2] aimed at constructing a physically distinguished self-adjoint realisation of the model. It was proved that if $|\nu| < 1$, there is only one self-adjoint extension whose functions in the domain are in $H^{1/2} \cap D(\gamma^{-1/2})$. Physically this requirement amounts to having finite expectation of both kinetic and potential energy. In the literature it is customary to refer to this particular self-adjoint realisation as the distinguished extension. In the work [22] I reviewed the history of the problem and the main ideas of the proofs.

We can distinguish among three regimes:

- the subcritical regime $|\nu| \leq \sqrt{\frac{3}{2}}$, where the minimal operator is essentially self-adjoint;
- the critical regime $\sqrt{\frac{3}{2}} < |\nu| < 1$, where the radial operator has a one real parameter family of self-adjoint realisations and there exists a distinguished one in the sense above mentioned.
- the overcritical regime, where the deficiency indices depend on $|\nu|$ and no distinguished extension exists.

Only a few works of the existing literature on Dirac-Coulomb operators were concerned with the classification of its self-adjoint extensions [56, 35] and both were based upon von Neumann’s theory.

In the work [25], together with A. Michelangeli, I applied instead the KVB theory to classify all the self-adjoint realisations of the radial Dirac-Coulomb operator in the critical regime. As it is well-known, Dirac-Coulomb operators are not semi-bounded but thanks to the presence of a spectral gap, i.e. $(-1, 1) \subseteq \sigma(A_{\min})$, we could apply Grubb’s version of KVB theory [32, Section 13] to classify the extensions. Working out resolvent formulas we could additionally produce a reliable estimate of the ground state of each extension.

All extensions turn out to have the same absolutely continuous spectrum, owing to Kuroda-Birman Theorem [52, Theorem 9.29 (ii)], since their resolvents differ by a rank-one operator from the resolvent of the distinguished extension.

As for the discrete spectra of the extensions, we classified them in the work [23] with A. Michenangeli. In particular, we solved explicitly the eigenvalue equation for the generic self-adjoint extension of the model and we explained how the two classical ways to compute eigenvalues, by means of supersymmetric methods [54, Sect. 5.5.2] (or the works [15, 31, 42, 53]) or truncation of series (see e.g. [10, Section 16]), select naturally two self-adjoint realisations only: the distinguished one and another one which we named the ‘mirror-distinguished’.

1.3. Pointlike perturbation of the hydrogen atom.

Delta-like perturbations play an important role both in mathematics, as they arise as suitable limits of actual Schrödinger operators; and in physics, as they provide solvable models for quantum systems subjected to highly concentrated impurities. In the non-relativistic model of the hydrogen atom delta-like perturbations supported in the nucleus arise, in the $c \rightarrow +\infty$ limit of the Dirac-Coulomb Hamiltonians as corrections of order $c^{-2}$ in the speed of light $c$ [9, Sections 33-34]. One of these terms is the so-called Darwin term and it is physically interpreted as an effective smearing out of the electrostatic interaction between the electron and the nucleus due to the Zitterbewegung, the rapid quantum oscillations of the electron.
The formal operator $H = -\Delta + \frac{\mu}{|x|^2} + \alpha \delta(x)$ is realised on $L^2(\mathbb{R}^3, dx)$ as an operator extension of $\hat{H} = -\Delta + \frac{\mu}{|x|^2}$ on $D(\hat{H}) = C^\infty_0(\mathbb{R}^3 \setminus \{0\})$. In fact, $\hat{H}$ turns out to be symmetric and to admit a one-parameter family of self-adjoint extensions.

Due to the radial symmetry of the problem one can reduce the study to the realisations of the $s$-wave radial operator. The literature on this problem dates back at least to Rellich [48] and to the subsequent works [62, 1, 13] where self-adjoint extensions are classified according to von Neumann’s scheme. In the work [24], in collaboration with A. Michelangeli, I reconsidered the problem applying KVB theory. In particular, we qualified explicitly the domain of the closure of the radial operator (which is the classical Sobolev space $H^2_0(\mathbb{R}^+)$) and of its Friedrichs extension.

In this case we also solved explicitly the eigenvalue equation in terms of Whittaker’s functions.

1.4. Geometric quantum confinement on Grushin-type manifolds.

When a quantum particle is constrained on an orientable Riemannian manifold $M$, one challenging problem that arises naturally is the question of the so-called geometric quantum confinement. The Hilbert space of the system is $L^2(M, d\mu_g)$, where $\mu_g$ is the volume form induced by the Riemannian metric on $M$, and the Schrödinger Hamiltonian of interest is a self-adjoint realisation of the operator $H = -\Delta_g + V$ where $-\Delta_g$ is the Laplace-Beltrami operator computed with respect to the measure $\mu$ and $V$ is a real-valued potential on $M$. Informally speaking, in this setting we have geometric quantum confinement when $-\Delta_g$ on $C^\infty_0(M)$ is essentially self-adjoint. Physically this means that the quantum particle does not reach the boundary of the manifold and hence it is confined by the geometry of the space and not by boundary conditions. In fact, boundary conditions encode an interaction of the boundary $\partial M$ with the particle localised in $M$ and if $C^\infty_0(M)$ is a domain of essential self-adjointness for $H$ it is natural to interpret this as a confinement in $M$ not due to the boundary (but to the sole geometry instead).

The case of smooth and geodesically complete Riemannian manifolds is relatively well-understood [21, 12]. For incomplete Riemannian manifolds the picture is less developed, yet fairly general classes of $V$’s are known which ensure the self-adjointness of Schrödinger operators on bounded domains of $\mathbb{R}^d$ with smooth boundary of co-dimension 1 [41] or more generally on bounded domains of $\mathbb{R}^d$ with non-empty boundary [57].

Quantum confinement on manifolds equipped with the so-called almost-Riemannian structure has attracted considerable attention over the last years [11, 45, 20].

In the work [28], in collaboration with A. Michelangeli and E. Pozzoli, I studied this problem in a class of two-dimensional incomplete Riemannian manifolds with metric of Grushin type, i.e.,

$$g_\alpha = dx \otimes dx + \frac{1}{|x|^{2\alpha}} dy \otimes dy$$

with $(x, y) \in (\mathbb{R} \setminus \{0\}) \times \mathbb{R}$ and $\alpha \in [0, +\infty)$. Calling $\mu_g$ the volume form associated with the metric $g_\alpha$, one can first simplify the problem by considering the splitting $L^2(\mathbb{R}^2, d\mu_g) = L^2(\mathbb{R}^- \times \mathbb{R}, d\mu_g) \oplus L^2(\mathbb{R}^+ \times \mathbb{R}, d\mu_g)$. The analysis of the essential self-adjointness boils down to the analysis of essential self-adjointness on each of the two reducing subspaces. Each of these subspaces can be written as constant-fibre direct integral as $L^2(\mathbb{R}^+ \times \mathbb{R}, d\mu_g) = \int_{\mathbb{R}^+} L^2(\mathbb{R}^+, dx) d\xi$ (and an analogous formula for $L^2(\mathbb{R}^-, d\mu_g)$). On each fibre we used Weyl’s criterion to fully characterise the regimes of presence and absence of essential self-adjointness of the associated Laplace-Beltrami operator (i.e., the regimes of presence or absence of quantum confinement).
In case $\alpha \in [0,1)$, the Laplace-Beltrami operator is not essentially self-adjoint and, with respect to the constant-fibre direct integral decomposition $L^2(\mathbb{R}^2, d\mu_g) = \int_{\mathbb{R}} (L^2(\mathbb{R}^-, d\nu) \oplus (L^2(\mathbb{R}^+, d\nu)) d\xi$, the minimal operator on each fibre has deficiency indices $(2, 2)$. To classify all its self-adjoint extensions we applied KVB theory and, reconstructing the constant fibre direct integrals of the same fibre extension for each $\xi \in \mathbb{R}$, we obtained five families of self-adjoint realisations of the Laplace-Beltrami operator on $M$. These families are characterised by having the same boundary condition for almost every $y \in \mathbb{R}$.

The properties of the dynamics generated by these families are different and, in particular, certain sub-families exhibit a disjoint dynamics (i.e., if the support of the wave-function at $t = 0$ is contained in one of the two half plane, there it remains for all times) and two of them exhibit mixed dynamics instead.

1.5. An integrable normal form for the Fermi-Pasta-Ulam problem.

Fermi-Pasta-Ulam (FPU) is nowadays referred to a set of physical models describing the dynamics of one-dimensional lattices with non-linear interactions. The classical FPU system is a classical (i.e., non-relativistic and non-quantum) system with nearest neighbour interaction and its Hamiltonian read

$$H(q, p) = \sum_{j=1}^{N} \left[ \frac{p_j^2}{2} + \phi(q_j - q_{j+1}) \right],$$

where $\phi(\xi) = \xi^2 + \alpha \xi^3 + \beta \xi^4 + O(\xi^5)$ is the potential energy term.

The interest for this problem arose in the 1950’s when it was used by E. Fermi, J. Pasta, S. Ulam and M. Tsingou to test the validity of the ergodic hypothesis in statistical physics [19].

They set up the first computer simulation in history to observe a paradoxical outcome: the systems did not show any ergodic behaviour. This is referred as FPU paradox.

Today it is known that the lack of ergodic behaviour of the generic particle chain on the short term is due to the vicinity of its dynamics to the integrable Toda chain, as first pointed out in [18] and further analysed in several subsequent investigations [8, 5, 3, 7]. Based on such works, we can draw the following phenomenological picture.

On a first time scale the system evolves very close to a Toda torus, and what is observed is nothing but an integrable deformation of the initial condition. Then, local chaos takes place on a second, longer time scale corresponding to the inverse of the largest Lyapunov exponent. The system reaches the final equilibrium state on the third, largest time scale. Such a scenario seems to be robust with respect to the choice of initial conditions, and certainly holds when smooth, i.e., long wavelength initial conditions are chosen. Indeed, in the case of smooth initial data, since the pioneering works of Kruskal and co-workers [61, 30], the dynamics of the system is well-known to be described by the Korteweg-de Vries equation (KdV), an integrable PDE.

The three time scales mentioned above are inverse powers of a certain small parameter (the specific energy in the numerical works).

In more recent studies [43, 44, 4, 6] it has been shown that an approximate description of the dynamics can be framed within the standard theory of normal forms. In particular it was proved that the resonant normal form of the Hamiltonian of the FPU consists, to leading order in a certain small parameter, of two KdV equations, one describing almost-right travelling waves and the other almost-left travelling waves. Such a result agrees with the perspective sketched above: the dynamics of the FPU chain on the short term turns out to be integrable. On the
other hand, many previous works [8, 5, 7] suggest that the normal form of the problem should be integrable as well to second order, but not to the third one.

In [29], in collaboration with A. Ponno and B. Rink, I found an explicit formal transformation that maps the FPU equations of motion into an integrable Hamiltonian (which is the sum of three Hamiltonians of the Korteweg-de Vries hierarchy) up to the second order in the small parameter.

In [49], we constructed explicitly the submanifold of left (or right) travelling waves to the third order in the small parameter

\[ h = N^{-1} \]

where \( N \) is the number of particles of the lattice. We then applied a refined version of the normal form transformation of [34] to show that the vector field of left/right travelling waves to third order in the small parameter is always in KdV hierarchy to order \( h^4 \) and to order \( h^6 \) only for particular choices of the parameters defining the particle interaction.

2. Forthcoming Research Projects

2.1. Explicit formulas for hydrogenoid eigenvalues.

As a follow-up of the work [24], we intend to investigate the eigenvalue equation for the generic self-adjoint realisation of a point-like perturbation of the hydrogen atom, the object of the activity described in paragraph 1.3. The eigenvalue equation is of the form

\[ \mathfrak{f}(E_n^{(\gamma)}) = \gamma \]

where \( \gamma \in \mathbb{R} \cup \{+\infty\} \) labels the self-adjoint realisations of the model, \( E_n^{(\gamma)} \) is the \( n \)-th eigenvalue of the self-adjoint operator labelled by \( \gamma \), and \( \mathfrak{f} \) is an explicit function. Due to the regularity of \( \mathfrak{f} \) it is possible to apply the implicit function theorem and get an approximate expression of \( E_n^{(\gamma)} \), the energy levels of the self-adjoint extension labelled with \( \gamma \), in terms of \( E_n^{(+\infty)} \), the energy levels of the hydrogen atom with respect to the parametrisation of [24]. A first question concerns the behaviour of the eigenvalues as \( \gamma \to +\infty \) i.e. when the self-adjoint extension is ‘close’ to the Friedrichs; a second question is the behaviour of the eigenvalues difference \( E_n^{(\gamma)} - E_n^{(+\infty)} \) with fixed \( \gamma \) and \( n \to +\infty \).

2.2. The Ehrenberg-Siday Effect.

Consider the Hamiltonian for a planar Dirac particle in \( \mathbb{R}^2 \) interacting with a magnetic field \( B \), described by the magnetic vector potential \( A \), \( B = \epsilon^{ij} \partial_i A^j \)

\[ H = \sigma \cdot (p - A) + \sigma_3 m. \]

By changing the gauge of the magnetic potential one sees that the operator is unitarily equivalent to the free Dirac operator acting on functions with the boundary condition \( \psi|_{\varphi=2\pi} = e^{-\Phi_i} \psi|_{\varphi=0} \).

The problem is inspired by [36] and it is possible to study it with the KVB theory. The main goal of the project is to classify a relevant sub-family of self-adjoint extensions of the operator on \( C_0^\infty (\mathbb{R}^2 \setminus \Gamma) \) with \( \Gamma = \{(x,y) \in \mathbb{R}^2 \mid y = 0, x \geq 0\} \). In this classification the Hamiltonians realising the Ehrenberg-Siday effect are included.

References


STATEMENT OF INTERESTS

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