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Stratified Spaces: Joining Analysis, Topology and Geometry

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Regularity of eigenfunctions of Schrödinger type equations

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(joint work with Catarina Carvalho, Victor Nistor)

In this talk we present some regularity statements for elliptic differential operators with singular potential, as for instance Schrödinger operators. The talk summarizes results from [1] which is work in collaboration with Catarina Carvalho and Victor Nistor. It is also intensively connected to collaborations with A. Ionescu and R. Lauter.

At first, we describe Lie manifolds, which were introduced in [3]. Roughly speaking the concept of a Lie manifold is a tool to compactify non-compact complete manifolds. A Lie manifold is a manifold with corners M (always with a fixed differentiable structure) and a fixed Lie algebra of vector fields which satisfies some axiomatic properties, for example we require that the Lie algebra of vector fields be a projective module over the ring $C^\infty(M)$. This Lie algebra of vector fields is used to describe a complete metric on the interior M_0 of M.

Examples of Lie manifolds are b-manifolds in the sense of Melrose, see e.g. [7], asymptotically hyperbolic manifolds and many similarly constructed manifolds. Euclidean space $\mathbb{R}^n$ is obtained from the scattering calculus [8].

We then describe a systematic way to conformally blow-up a Lie-manifold M along a given submanifold N. The blow-up construction consists of two parts: at first we obtain a new manifold with corners $[M : N]$. This part is quite standard, and also similar to [9]. We assume transversality at the boundary and $N \cap M_0 \neq \emptyset$. The second part is to specify a Lie algebra of vector fields on this blownn-up manifold $[M : N]$. A subtle step is to prove that the Lie algebra of vector fields is a projective module, and one of the most amazing aspects is that no condition on the behavior of the Lie algebra of vector fields on M is required for our construction. Associated to this new Lie algebra of vector fields there is a complete metric on the interior $[M : N]_0$ of $[M : N]$. This new metric on $[M : N]_0 \cong M_0 \setminus N$ is conformal to the original metric on M_0.

We apply this blow-up construction to the study of the eigenvalue equation for Schrödinger type operators $\mathcal{H}$. For example we study the classical Schrödinger operator $\mathcal{H} := -\Delta + V$ of a k-electron atom with

$$V(x) = \sum_{1 \leq j \leq k} \frac{b_j(x)}{|x_j|} + \sum_{1 \leq i < j \leq k} \frac{c_{ij}(x)}{|x_i - x_j|}, \tag{1}$$

where $x = (x_1, x_2, \ldots, x_k) \in \mathbb{R}^{3k}$, $x_j \in \mathbb{R}^3$, and b_j and c_{ij} are suitable smooth functions. Another example would be a molecule, where we consider the nuclei as very heavy and thus with a fixed position.

The blow-up construction described above will be applied now. We start with euclidean space $\mathbb{R}^{3k}$ equipped with the Lie manifold structure from the scattering calculus. The Schrödinger operator defines a structure of a stratified space on $\mathbb{R}^{3k}$. The highest dimensional strata are those where exactly two particles meet, and these strata have codimension 3. The lowest stratum is where the number of meeting particles is maximal, and it is typically a single point. The Schrödinger operator has a singular potential along the strata, in the sense that the potential is unbounded in the neighborhood of the strata. Our blow-up construction now blows up the lowest-dimensional stratum first, and then iteratively the strata of higher and higher dimension. During this blow-up-construction the eigenvalue equation for the Schrödinger operator is translated into an equation which remains "bounded with respect to the blown-up metric" in a neighborhood of the strata.

This allows us to apply regularity statements for Lie manifolds, developed in [2]. In this way we obtain the following regularity result for the eigenfunctions of the Schrödinger equation. To express this result we define the Babuška-Kondratiev spaces .

$$\mathcal{K}_a^m(\mathbb{R}^{3k}, r_S) := \{u : \mathbb{R}^{3k} \to \mathbb{C} \mid r_S^{|\alpha|-a} \partial^\alpha u \in L^2(\mathbb{R}^{3k}),\ |\alpha| \leq m\}, \tag{2}$$

where $a \in \mathbb{R}$ and $m \in \mathbb{N}$. The weight function $r_S(x)$ is the smoothed distance from x to the singular strata, however the distance r_S is not measured with respect to euclidean distance, but with respect to a metric on the ball compactification of $\mathbb{R}^{3k}$. This modified choice does not effect $\mathcal{K}_a^m(\mathbb{R}^{3k}, r_S)$ on closed balls, but it does globally.

Theorem 1 ([1, Theorem 4.3])**.** *Assume $u \in L^2(\mathbb{R}^{3k})$ is an eigenfunction of the single-nucleus k-electron Schrödinger operator, then*

$$u \in \mathcal{K}_a^m(\mathbb{R}^{3k}, r_S)$$

for all $m \in \mathbb{N}$ *and for all* $a \leq 0$.

This results is mainly interesting close to the strata of non-maximal dimension. The result is already known for the classical Schrödinger operator locally along the top-dimensional strata, in fact it follows from recent research by Fournais [6] in which it is shown that the eigenfunction satisfies some modified version of analyticity. Our result is stronger close to those places where at least three particles meet. The approach in [6] is also more retrictive than ours, in particular as it requires analyticity of the potential, which we do not assume.

In current work we modify the blow-up construction, and we expect to obtain a version of the above theorem in which r_S is replaced by the euclidean distance to the singular stratum. It also seems likely to us that the coefficient a in the above theorem can be improved to all $a < 3/2$. One motivation to conjecture this is that the corresponding statement holds for the Schrödinger operator associated to several nuclei and a single electron.

Theorem 2 ([1, Theorem 4.6]). *Let* $u \in L^2(\mathbb{R}^3)$ *be such that* $\mathcal{H}u = \lambda u$*, in distribution sense. Then* $u \in \mathcal{K}_a^m(\mathbb{R}^3, r_S)$ *for all* $m \in \mathbb{N}$ *and all* $a < 3/2$.

Finally we also want to mention interesting developments by Flad, Harutyunyan, Schneider, and Schulze, see [5, 4]. Their approach is partially related to ours, but has different goals, in particular they obtain precise asymptotic developments for systems with few particles.

References

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