

# Open problems about many-body Dirac operators

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Recently, I exchanged a series of interesting email letters with a colleague from the Faculty of Chemistry, University of Warsaw, Prof. Bogumił Jeziorski. In these letters, Jeziorski formulated two interesting mathematical questions, which I would like to share with the readers of the Bulletin of the IAMP. Below, with the author's consent, I give an English translation of large parts of Jeziorski's letters.

*Let us consider the essential self-adjointness of the Dirac-Coulomb operator  $H_{\text{DC}}$  for a helium-like ion. This operator has the form*

$$H_{\text{DC}} = D(1, Z) + D(2, Z) + 1/|\mathbf{r}_1 - \mathbf{r}_2|,$$

*where*

$$D(i, Z) := c\vec{\alpha}\vec{p}_i + m\beta - Z/|\mathbf{r}_i|,$$

*$i = 1, 2$ , is the usual Dirac operator for an electron  $i$  in a hydrogen-like ion of charge  $Z$  and  $\mathbf{r}_i$ ,  $i = 1, 2$ , is the vector describing the position of the  $i$ th electron. (In the system of units used here, the speed of light  $c$  coincides with the inverse of the fine structure constant,  $\alpha \approx 1/137.036$ ).*

*It is well-known that the operator  $D(i, Z)$  is essentially self-adjoint for  $|Z| < \sqrt{3}/(2\alpha)$ , although the Kato-Rellich Theorem proves this only for  $|Z| < 1/(2\alpha)$ . For  $|Z| > \sqrt{3}/(2\alpha)$  there exist many self-adjoint extensions. For  $|Z| < 1/\alpha$  there exists a distinguished self-adjoint extension, which can be adopted as the physical one [20].*

*I think that adding  $1/|\mathbf{r}_1 - \mathbf{r}_2|$  will not change the situation in an essential way and the Kato-Rellich Theorem will easily imply the essential self-adjointness of  $H_{\text{DC}}$ . Unfortunately, I was not able to find a proof of this statement in the mathematical literature. Perhaps, mathematicians view this as a rather easy generalization of Kato's proof for a nonrelativistic Helium atom.*

*I believe the operator  $H_{\text{DC}}$  has a continuous spectrum from  $-\infty$  to  $\infty$ . It would be very important to prove that there are no eigenvalues (corresponding to square integrable eigenfunctions) embedded in this continuous spectrum.*

I am not an expert in mathematical properties of many-body Dirac operators. There are a number of researchers (notably in Paris and Munich), who studied them and wrote interesting rigorous papers on this subject, such as [17, 3, 6]. However, I doubt whether a proof of either conjecture formulated in the letter of Jeziorski exists in the literature. I agree with him that these conjectures are plausible, interesting mathematically and well-motivated physically. They are well posed mathematically – they could be understood and appreciated even by a mathematician without a physical background.

The proof of the essential self-adjointness of the usual many-body Schrödinger operator with Coulomb interactions that I know [14] uses in an essential way the fact that the kinetic energy is quadratic in the momenta and is bounded from below. Dirac and many-body Dirac operators do not have these properties. Therefore, the usual proof of the essential self-adjointness does not generalize from the many-body Schrödinger to the many-body Dirac case. After discussing the problem briefly with some of my colleagues I realized that I even do not know how to prove the essential self-adjointness in the case  $Z = 0$ !

Our understanding of embedded point spectrum is even more limited. To my recollection, for many-body Schrödinger operators one can show the absence of positive eigenvalues [4] and the absence of embedded eigenvalues

for generic localized interactions [1]. I do not know similar results for many-body Dirac operators. Let me quote again from a letter of Jeziorski.

*Obviously, it would be more important to prove that  $H_{\text{DC}}$  has no eigenvalues [than to show its essential self-adjointness]. The Hamiltonian  $H_{\text{DC}}$  is used by chemists in hundreds of papers every year and with a tacit assumption that it has square integrable eigenfunctions. If one could prove that there are no such functions, I think that such a paper could be cited many times a year. I am somewhat surprised that mathematicians proved lots of difficult theorems on one-particle Dirac operators with singular potentials and, as it seems, were not interested in a system of two electrons with realistic potentials (...)*

*If the singularity  $1/|\mathbf{r}_i|$  is difficult, it could be regularized (which amounts to a finite nucleus model). If the singular nature of  $1/|\mathbf{r}_1 - \mathbf{r}_2|$  causes problems, one could regularize this function as well, although this is much less justified physically. If such a regularization works and the resulting  $H_{\text{DC}}$  is easily shown to be essentially self-adjoint, it only remains to prove the absence of point spectrum. Perhaps this would work?*

A separate question arises: what is the physical relevance of many-body Dirac-Coulomb operators? To my understanding, many-body Dirac operators are postulated in chemistry and physics ad hoc, by analogy with many-body Schrödinger operators.

Many-body Schrödinger operators are well justified as Hamiltonians describing nonrelativistic matter. Note, in particular, that they are covariant with respect to the basic group of nonrelativistic physics – the Galilean group. It should be possible to derive many-body Schrödinger operators with Coulomb interactions as low-energy effective Hamiltonians from the full QED. (Of course, the full QED has well-known mathematical problems – it is believed to exist only as a perturbative theory. But this is another question).

The status of interacting many-body Dirac operators is much more shaky. They are not bounded from below, which indicates that they are not Hamiltonians of quantum dynamics. Unfortunately, they have another serious flaw: they are not covariant with respect to the Poincaré group. Perhaps, they describe approximately the time evolution of some time-ordered Green's functions. Maybe they appear in a certain natural approximate version of the Bethe-Salpeter equation.

Nonrelativistic many-body quantum mechanics is a difficult theory, but at least it is based on solid foundations – the many-body Schrödinger Hamiltonian. When one tries to generalize it to the relativistic setting, one seems essentially forced to adopt the point of view of quantum field theory. Unfortunately, the bound-state problem in quantum field theory is poorly understood.

There exists, however, a class of relativistic many-body problems where apparently a rather systematic and successful theory exists. This class includes few-body systems such as the positronium, hydrogen-like, helium-like, or even lithium-like ions. The most famous example of this category is the so-called Lamb shift. To my knowledge, there exist systematic perturbative methods to compute energy levels of such system. They always need a small parameter – usually the fine structure constant  $\alpha$ , sometimes also  $1/Z$  and the ratio of electron to nucleus mass. Non-perturbative QED is not known, probably it does not exist.

Note, however, that energy levels are not computed as eigenvalues of a self-adjoint Hamiltonian. They are defined as the position of the poles of Green's functions [11], or are derived from the adiabatic  $S$ -matrix formalism of Gell-Mann–Low [9]. In particular, they usually have a non-vanishing imaginary part describing the width of the resonance. Computations of few-particle relativistic energy levels are a specialty of another colleague of mine, Krzysztof Pachucki from the Institute of Theoretical Physics (Faculty of Physics, University of Warsaw). Pachucki taught me that systematic computations of these problems do not involve the many-body Dirac Hamiltonian, but rather the many-body Schrödinger Hamiltonian. Interesting examples of such results are contained in two recent papers by a group of researchers including Jeziorski and Pachucki [7, 13] devoted to molecular hydrogen, which is a few-body system, with 2 heavy and 2 light constituents. The analysis contained in these papers starts from a 4-body Schrödinger operator, with computations that go beyond the Born-Oppenheimer approximation and then include relativistic corrections. Jeziorski writes:

*We are especially proud of Fig 3 in [7], which shows the QED effects in the molecular spectrum determined experimentally and their comparison with our theoretical prediction –first such observations in the literature.*

[Fig. 3 shows QED contributions to the rotational excitation energies of molecular hydrogen for the zero vibrational number – comparison of the the-

oretical calculations (open diamonds) with the experimental data. Almost all diamonds fall well inside the vertical bars denoting experimental uncertainties].

Let me quote again Jeziorski:

*I would like to note that I am not involved in solving the Dirac-Coulomb equation. In our computations based on QED this equation does not appear. However, it is the foundation of the so-called “relativistic quantum chemistry”, because the majority of chemists do not realize that it cannot have a pure point spectrum. In my opinion, it does not have a pure point spectrum, and its absence is beyond any doubt (Pachucki has the same opinion). On the other hand, chemists can say that since there is no mathematical proof, they can have doubts! There exists, however, strong numerical evidence – the so-called Brown-Ravenhall disease (BRD) [2], called also the “continuum dissolution”, and three papers from Jacek Karwowski’s group in Toruń [12], where for the first time the width of the resonance modeling the ground state of the helium atom was computed. As a proof of the strength of the faith in the existence of eigenvalues of the Dirac-Coulomb Hamiltonian let me mention that in a recent monograph [15] one can find a statement “continuum dissolution has never been observed in actual calculations”. Another influential monograph [5] views the destructive effect of BRD as only “alleged”. It should be mentioned, however, that the significance of the results of Refs. [12] has been recently noticed in the chemical literature [8].*

I am greatly surprised that the belief in the existence of embedded point spectrum of Dirac-Coulomb operators is so widespread. I have always thought that every physicist or mathematician who played a little with the perturbation theory for operators has developed the intuition that embedded eigenvalues are an exceptional, non-generic phenomenon that needs special circumstances to happen. (This does not mean that it should be easy to prove their absence in concrete situations).

Jeziorski sent me a very recent review paper [10] of Wenjian Liu, an authority in relativistic quantum chemistry, suggesting to read page 4 of this paper. It appears that Liu does not believe that the DC equation has no eigenvalues. Liu discusses the results of [12], trying to find a flaw in it. Here is an excerpt of Liu’s paper:

*Therefore, it cannot be excluded that the the complex energies obtained by Pestka et al [12] are due to incompleteness errors in the basis set. Given such uncertainties, the conclusion that the DC Hamiltonian has no bound states may be premature. What can really be concluded at this stage is that the BRD is much less virulent than originally claimed, and that the no-pair projection, as recommended by Sucher, for avoiding the BRD, is not really needed.*

The many-body Dirac equation is used by many chemists. Apparently, they have some success in predicting properties of atoms and molecules. Here again a comment of Jeziorski:

*They [chemists that use the Dirac-Coulomb equation] obtain good numbers, because for heavy atoms the Dirac-Coulomb model is much better than the Schrödinger model, in spite of its artifacts. This is because the widths of resonances of the DC equation (which model bound states) are apparently of the order of  $Z^3\alpha^3$ , and the relativistic corrections from DC equation scale as  $Z^4\alpha^2$  [both relative to the nonrelativistic energy  $m\alpha^2$ .] The ratio of the (non-physical) resonance width to the relativistic correction is therefore  $\alpha/Z$ . Additionally, the error involved in solving the DC equation (which amounts to finding the resonances) is much bigger than their width. Most cases of the agreement with experiments belong to structural chemistry and thermochemistry, where experimental errors are much bigger than  $Z^3\alpha^3$  (but often smaller than  $Z^4\alpha^2$ ).*

Sometimes it is claimed [19] that in quantum chemistry one should not use the many-body Dirac operator itself, but its compression  $PH_{\text{DC}}P$ , where

$$P = P_1 \otimes P_2 \dots \otimes P_N,$$

$N$  is the number of electrons and  $P_i$  is the orthogonal projection onto one-electron states of “positive energy”. The advantage of the “Sucher’s no-pair Hamiltonian”  $PH_{\text{DC}}P$  is its boundedness from below. However, in order to determine the projections  $P_i$  one needs to adopt a certain 1-electron potential, which is to a large extent arbitrary. In practice, the operators  $PH_{\text{DC}}P$  seem to be mostly used in intermediate steps when eigenvalues of the unprojected operator  $H_{\text{DC}}$  are computed.

Anyway, together with Jeziorski, I believe that, most likely, what chemists compute are not true eigenvalues of the many-body Dirac-Coulomb operator, but its resonances. This leads to a nontrivial question what is a mathematical definition of a resonance.

There exists a satisfactory definition of a resonance for many-body Schrödinger operators. As it is well-known, they are eigenvalues of the operator distorted by dilation analyticity. Equivalently, they can be defined as poles of the resolvent between dilation analytic vectors.

For one-body Dirac-Coulomb operators the dilation analyticity approach goes through [21, 16]. For many-body Dirac-Coulomb operators apparently it is difficult to apply this approach rigorously [18], even though it is used in numerical studies in the 2-body case in [12].

Thus, there are two problems that I do not understand. Unfortunately, these problems are quite vague – they are not as rigorously formulated as Jeziorski’s questions.

– What is a good definition of a resonance for many-body Dirac-Coulomb operators?

– What is a physical justification (that essentially means, a derivation from QED) of applications of many-body Dirac-Coulomb operators to atoms and molecules?

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