Dirac operators with electrostatic δ-shell interactions: spectral and scattering properties

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in collaboration with *Jussi Behrndt*, *Markus Holzmann*, and *Vladimir Lotoreichik*

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Once upon a time

The problem has a history: deep in the last century we wrote a paper

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in which we discussed *singular Dirac operators* formally written as

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Then there was a *long silence* followed by a recent *burst of activity* in Bilbao, Graz, Prague, and elsewhere, bringing in *a lot more generality.*

Well, not exactly a sleeping beauty

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This not the three-dimensional massive one we speak about here, but on the other hand, it makes perfect sense to investigate such particles confined to regions of an *arbitrary shape*, see for instance

- R.D. Benguria, S. Fournais, E. Stockmeyer, H. Van Den Bosch: Self-adjointness of two-dimensional Diracoperators on domains, *Ann. Henri Poincaré* **18** (2017), 1371–1383.
- R.D. Benguria, S. Fournais, E. Stockmeyer, H. Van Den Bosch: Spectral gaps of Dirac operators describing graphene quantum dots, *Math. Phys. Anal. Geom.* **20** (2017), 11 (12pp).

Quasi boundary triples

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Let T be a linear operator in $\mathfrak{H}$ such that $\overline{T} = S^*$, then $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called a *quasi boundary triple* for S^* if $(\mathcal{G}, (\cdot,\cdot)_{\mathcal{G}})$ is a Hilbert space and $\Gamma_0, \Gamma_1 : \mathrm{dom}\, T \to \mathcal{G}$ are linear maps satisfying the following conditions:
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(i) The abstract Green's identity

$$(Tf, g)_{\mathfrak{H}} - (f, Tg)_{\mathfrak{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}}$$

is valid for all $f, g \in \mathrm{dom}\, T$.

(ii) The range of the mapping $\Gamma = (\Gamma_0, \Gamma_1)^\top : \mathrm{dom}\, T \to \mathcal{G} \times \mathcal{G}$ is dense.

(iii) The operator $H_0 := T \upharpoonright \ker \Gamma_0$ is self-adjoint in $\mathfrak{H}$.

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Such a triple is said to be a *generalized boundary triple* if $\mathrm{ran}\, \Gamma_0 = \mathcal{G}$ and an *ordinary boundary triple* if $\mathrm{ran}\, \Gamma = \mathcal{G} \times \mathcal{G}$.

J. Behrndt, M. Langer: Boundary value problems for elliptic partial differential operators on bounded domains, *J. Func. Anal.* **243** (2007), 536–565.

The γ field and the Weyl function M

Given a quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ we define them as

$$\rho(A_0) \ni \lambda \mapsto \gamma(\lambda) = \big(\Gamma_0 \restriction \ker(T-\lambda)\big)^{-1},$$

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They allow us to construct extensions: for $B \in \mathfrak{B}(\mathcal{G})$ we consider

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For ordinary boundary triples one usually writes $\ker(\Gamma_1 - \Theta\Gamma_0)$ and the operator $\Theta = -B^{-1}$ determines a unique extension. When dealing with quasi boundary triples, more caution is needed.

A Krein-type formula

Theorem

Let S and $\overline{T} = S^*$ be as above with a quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ and $A_0 = T \upharpoonright \ker \Gamma_0$. Let further $A_{[B]}$ be the extension of S corresponding to an operator B. Then for all $\lambda \in \rho(A_0)$ one has

$$\ker(A_{[B]} - \lambda) = \{\gamma(\lambda)\varphi : \varphi \in \ker(I + BM(\lambda))\}$$

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in particular, $\lambda \in \sigma_{\rm p}(A_{[B]})$ holds if and only if if $-1 \in \sigma_{\rm p}(BM(\lambda))$. Furthermore, if $\lambda \in \rho(A_0)$ is not an eigenvalue of $A_{[B]}$ then we have

(i) $g \in \operatorname{ran}(A_{[B]} - \lambda)$ *if and only if* $B\gamma(\overline{\lambda})^* g \in \operatorname{dom}(I + BM(\lambda))^{-1}$;

(ii) *For all* $g \in \operatorname{ran}(A_{[B]} - \lambda)$ *we have*

$$(A_{[B]} - \lambda)^{-1} g = (A_0 - \lambda)^{-1} g - \gamma(\lambda)\big(I + BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^* g.$$

If $B \in \mathfrak{B}(\mathcal{G})$ is self-adjoint and $(I + BM(\lambda_\pm))^{-1} \in \mathfrak{B}(\mathcal{G})$ for some $\lambda_\pm \in \mathbb{C}^\pm$, then $A_{[B]}$ is a self-adjoint operator in $\mathfrak{H}$ and the formula holds for all $\lambda \in \rho(A_0) \cap \rho(A_{[B]})$ and all $g \in \mathfrak{H}$.

J. Behrndt, M. Langer, V. Lotoreichik: Trace formulae and singular values of resolvent power differences of self-adjoint elliptic operators, *J. London Math. Soc.* **88** (2013), 319–337.

Application to singular Dirac operators

We start from the free Dirac operator

$$H_0 f := -ic \sum_{j=1}^{3} \alpha_j \partial_j f + mc^2 \beta f, \quad \mathrm{dom}\, H_0 = H^1(\mathbb{R}^3; \mathbb{C}^4),$$

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Its resolvent is know to act as $(H_0 - \lambda)^{-1} f(x) = \int_{\mathbb{R}^3} G_\lambda(x-y) f(y) \mathrm{d}y$, where the $\mathbb{C}^{4\times 4}$-valued integral kernel G_λ is given by

$$G_\lambda(x) = \left(\frac{\lambda}{c^2} I_4 + m\beta + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} - (mc)^2} |x| \right) \frac{i}{c|x|^2} \alpha \cdot x \right) \frac{e^{i\sqrt{\lambda^2/c^2 - (mc)^2}|x|}}{4\pi |x|}.$$

B. Thaller: *The Dirac Equation*, Texts and Monographs in Physics, Springer, Berlin 1992.

Quasi boundary triples

Given a bounded C^∞-domain in $\mathbb{R}^3$ with the boundary Σ, we introduce

$$\gamma\varphi(x) := \int_\Sigma G_0(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \mathbb{R}^3,\ \varphi \in L^2(\Sigma; \mathbb{C}^4),$$

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which is bounded and everywhere defined, and furthermore, we define the strongly singular integral operator $M : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ by

$$M\varphi(x) := \lim_{\varepsilon \searrow 0} \int_{|x-y|>\varepsilon} G_0(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \Sigma,\ \varphi \in L^2(\Sigma;\mathbb{C}^4).$$

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$$\Gamma_0(f+\gamma\varphi) = \varphi \quad \text{and} \quad \Gamma_1(f+\gamma\varphi) = f|_\Sigma + M\varphi, \quad f+\gamma\varphi \in \mathrm{dom}\, T,$$

is a quasi boundary triple for $\overline{T} = S^*$ and $T \upharpoonright \ker\Gamma_0$ coincides with H_0.

The γ field and the Weyl function M

These quantities, $\gamma(\lambda)$ and $M(\lambda)$, associated with the quasi boundary triple $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ are obtained *by replacing $G_0(x)$ by $G_\lambda(x)$* in the above formulæ

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properties of these operator-valued functions are derived, in particular

(i) The limits $M(\pm mc^2):=\lim_{\lambda\to\pm mc^2}M(\lambda)$ exist in the operator norm on $\mathfrak{B}\big(L^2(\Sigma;\mathbb{C}^4)\big)$ and can be expressed by means of the 'localized convolution' with $G_{\pm mc^2}(x)$.

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(ii) $\lambda\mapsto M(\lambda)$ is uniformly bounded on the spectral gap, i.e.

$$M_0:=\sup_{\lambda\in[-mc^2,mc^2]}\|M(\lambda)\|<\infty.$$

Further properties of $\gamma(\lambda)$ and $M(\lambda)$

Furthermore, we have

(i) For any $\lambda \in \rho(H_0)$ there exists a *compact* $K(\lambda)$ in $L^2(\Sigma; \mathbb{C}^4)$ such that

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(ii) With the M_0 defined above, there exists an *at most countable family* of functions $\mu_n : [-mc^2, mc^2] \to \left[\frac{1}{4c^2 M_0}, M_0\right]$, continuous and non-decreasing, such that such that

$$\sigma(M(\lambda)) = \left\{\pm\frac{1}{2c}\right\} \cup \{\mu_n(\lambda) : n \in \mathbb{N}\} \cup \left\{-\frac{1}{4c^2 \mu_n(\lambda)} : n \in \mathbb{N}\right\}.$$

Moreover, for any fixed $\lambda \in [-mc^2, mc^2]$ the number $\frac{1}{2c}$ is the only possible accumulation point of the sequence $(\mu_n(\lambda))$.

Electrostatic shell interaction

Consider now self-adjoint extension for which B is a *scalar operator*, in other words, for a given Σ and $\eta \in \mathbb{R} \setminus \{\pm 2c\}$ we put

$$H_\eta := T \upharpoonright \ker(\Gamma_0 + \eta\Gamma_1),$$

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The above results about the properties the γ-field and Weyl function $M(\cdot)$ allow us to determine spectral properties of H_η.

Spectral properties of H_η

Theorem

Let $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0,\Gamma_1\}$ *be the quasi boundary triple described above with the corresponding* γ*-field* $\gamma(\cdot)$ *and Weyl function* $M(\cdot)$*. Then the Dirac operator* H_η *is self-adjoint in* $L^2(\mathbb{R}^3;\mathbb{C}^4)$ *for any* $\eta\in\mathbb{R}\setminus\{\pm 2c\}$ *and*

$$(H_\eta-\lambda)^{-1}=(H_0-\lambda)^{-1}-\gamma(\lambda)\big(I_4+\eta M(\lambda)\big)^{-1}\eta\gamma(\bar{\lambda})^*$$

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Adding a Lorentz scalar

While I have electrostatic interaction in the title, let me briefly mention what happens if the interaction combined with a *Lorentz δ shell*, i.e.

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$$\frac{1}{2}(\eta I_4 + \tau\beta)\,(h_+ + h_-) = -\frac{i\alpha\cdot\nu}{c}\,(h_+ - h_-).$$

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Remark: Other shell interaction have been considered, e.g., the one give by $H_{\eta,\theta} = H_0 + (\eta + \theta(\alpha\cdot\nu))\delta_\Sigma(x)$

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Remark: Other shell interaction have been considered, e.g., the one give by $H_{\eta,\theta} = H_0 + (\eta + \theta(\alpha\cdot\nu))\delta_\Sigma(x)$; for particular values of η, θ they are unitarily equivalent to a separating $H_{\eta'}$ by a gauge transformation

A. Mas: Dirac operators, shell interactions, and discontinuous gauge functions across the boundary, *J. Math. Phys.* **58** (2017), 022301.

The meaning of such interactions

In the nonrelativistic case the δ-shell interaction can be regarded as an *idealization of a high and narrow potential barrier* (or a deep well) which is expressed by the *norm-resolvent convergence*

$$-\Delta + \frac{1}{\varepsilon} V\left(\frac{u_x}{\varepsilon}\right) \longrightarrow -\Delta + \alpha\delta_\Sigma(x) \quad \text{as } \varepsilon \to 0\,,$$

where $u_x := \mathrm{dist}(x, \Sigma)$ and $\alpha := \int V(u)\,\mathrm{d}u$.

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For Dirac operators we have a similar approximation results, however, with an important difference: the approximation family of potentials *scales in a nonlinear way* which is an effect related to *Klein's paradox*

P. Šeba: Kleins paradox and the relativistic point interaction, *Lett. Math. Phys.* **18** (1989), 77–86.

A. Mas, F. Pizzichillo: Klein's paradox and the relativistic δ-shell interaction in $\mathbb{R}^3$, *Annal. & PDE* **11** (2018), 705–744.

An isoperimetric inequality

Returning to the purely electrostatic case, we note that the critical value depends on the geometry of Σ.

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Theorem

Let $\Sigma = \partial\Omega$ *and* $C_\pm(\Sigma) = 4\left(\pm\, mc^2 \frac{\mathrm{Area}(\Sigma)}{\mathrm{Cap}(\Omega)} + \sqrt{m^2c^4 \left(\frac{\mathrm{Area}(\Sigma)}{\mathrm{Cap}(\Omega)}\right)^2 + \frac{1}{4}}\right)$

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$$\sup\left\{|\eta| : \sigma_{\mathrm{disc}}(H_\eta) \neq \emptyset\right\} \geq C_+(\Sigma) \quad \text{and} \quad \inf\left\{|\eta| : \sigma_{\mathrm{disc}}(H_\eta) \neq \emptyset\right\} \leq C_-(\Sigma)$$

In both cases, the equality holds if and only if Ω *is a ball.*

N. Arrizabalaga, A. Mas, L. Vega: An isoperimetric-type inequality for electrostatic shell interactions for Dirac operators, *Commun. Math. Phys.* **344** (2016), 483–505.

A related result

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If $\Sigma = S_R$ is a *sphere*, $\sigma_{\mathrm{disc}}(H^{\mathrm{nr}}_{\eta,\Sigma}) \neq \emptyset$ holds if $-\eta R > 1$.

J.-P. Antoine, F. Gesztesy, J. Shabani: Exactly solvable models of sphere interactions in quantum mechanics, *J. Phys. A: Math. Gen.* **20** (1987), 3687–3712.

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Suppose that the coupling is *critical*, i.e. $\eta R = -1$, and ask whether *deformations of Σ produce a discrete spectrum*:

- if the deformation is *area-preserving*, the claim holds *locally*, but not globally

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If $\Sigma = S_R$ is a *sphere*, $\sigma_{\mathrm{disc}}(H^{\mathrm{nr}}_{\eta,\Sigma}) \neq \emptyset$ holds if $-\eta R > 1$.

J.-P. Antoine, F. Gesztesy, J. Shabani: Exactly solvable models of sphere interactions in quantum mechanics, *J. Phys. A: Math. Gen.* **20** (1987), 3687–3712.

Suppose that the coupling is *critical*, i.e. $\eta R = -1$, and ask whether *deformations of Σ produce a discrete spectrum*:

- if the deformation is *area-preserving*, the claim holds *locally*, but not globally
- if the deformation is *capacity-preserving*, the claim *holds generally*

P.E., M. Fraas: On geometric perturbations of critical Schrödinger operators with a surface interaction, *J. Math. Phys.* **50** (2009), 112101 (12pp).

The critical case

In case of the critical coupling, $\eta = \pm 2$, spectral properties are different:

Theorem

The operators $H_{\pm 2}$ are self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ and their domains are not contained in $H^1(\mathbb{R}^3;\mathbb{C}^4)$. As before,

$$\sigma_{\mathrm{ess}}(H_{\pm 2}) \supset (-\infty, mc^2] \cup [mc^2, \infty),$$

however, the inclusion is in general sharp. In particular, if Σ contains a flat part, we have $0 \in \sigma_{\mathrm{ess}}(H_{\pm 2})$.

J. Behrndt, M. Holzmann: On Dirac operators with electrostatic δ-shell interactions of critical strength, *J. Spect. Theory*, to appear; `arXiv:1612.02290`

Another proof of the self-adjointnes together with the observation that *zero belongs to the spectrum when σ is a plane* can be found in

N. Arrizabalaga, A. Mas, L. Vega: Shell interactions for Dirac operators, *J. Math. Pures at Appliquées* **102** (2014), 617–639.

A trace class property

Let us return to the non-separated case and look at it now from the *scattering point of view*:

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$$\mathrm{tr}\left[(H_\eta - \lambda)^{-3} - (H_0 - \lambda)^{-3}\right] = -\frac{1}{2}\mathrm{tr}\left[\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}\left((I_4 + \eta M(\lambda))^{-1}\eta\frac{\mathrm{d}}{\mathrm{d}\lambda}M(\lambda)\right)\right]$$

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holds. In particular, the wave operators for the pair $\{H_\eta, H_0\}$ exist and are complete, and consequently, the absolutely continuous parts of H_η and H_0 are unitarily equivalent.

J. Behrndt, P.E., M. Holzmann, V. Lotoreichik: On the spectral properties of Dirac operators with electrostatic δ-shell interactions, *J. Math. Pures at Appliquées* **111** (2018), 47–78.

The nonrelativistic limit

Recall the the singular Schrödinger operator mentioned above,

$$H_\eta^{\mathrm{nr}} = -\Delta + \eta\delta(x - \Sigma)$$

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$$\mathfrak{b}_{\alpha,\Gamma}[f] := \frac{1}{2m}\|\nabla f\|^2_{L^2(\mathbb{R}^3;\mathbb{C}^3)} + \eta\|f|_\Sigma\|^2_{L^2(\Sigma;\mathbb{C})}, \quad \mathrm{dom}\,\mathfrak{b}_{\alpha,\Gamma} = H^1(\mathbb{R}^3;\mathbb{C})$$

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What is important, we can expressed its resolvent using the free one,

$$\left(-\frac{1}{2m}\Delta - \lambda\right)^{-1} f(x) = \int_{\mathbb{R}^3} K_\lambda(x-y)f(y)\mathrm{d}y, \quad x \in \mathbb{R}^3,\ f \in L^2(\mathbb{R}^3;\mathbb{C}),$$

where

$$K_\lambda(x) := 2m\,\frac{e^{i\sqrt{2m\lambda}|x|}}{4\pi|x|}, \quad x \in \mathbb{R}^3 \setminus \{0\}.$$

The resolvent of H_α^{nr}

To this aim, we define the operators $\widetilde{\gamma}(\lambda) : L^2(\Sigma;\mathbb{C}) \to L^2(\mathbb{R}^3;\mathbb{C})$,

$$\widetilde{\gamma}(\lambda)\varphi(x) := \int_\Sigma K_\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \mathbb{R}^3,\ \varphi \in L^2(\Sigma;\mathbb{C}),$$

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Theorem

Let $\alpha \in \mathbb{R}$ and $\lambda \in \mathbb{C}\setminus\mathbb{R}$, then the operator $I + \eta\widetilde{M}(\lambda)$ has a bounded and everywhere defined inverse and

$$(H_\alpha^{\mathrm{nr}} - \lambda)^{-1} = \left(-\frac{1}{2m}\Delta + \lambda\right)^{-1} - \widetilde{\gamma}(\lambda)\big(I + \eta\widetilde{M}(\lambda)\big)^{-1}\eta\widetilde{\gamma}(\overline{\lambda})^*.$$

J.F. Brasche, P.E., Yu.A. Kuperin, P. Šeba: Schrödinger operators with singular interactions, *J. Math. Anal. Appl.* **184** (1994), 112–139.

The nonrelativistic limit

To compare the two Hamiltonians, we have restrict the relativistic one to the positive energy subspace associated with the projection

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Theorem

Let $\pm 2c \neq \eta \in \mathbb{R}$ and let H_η be the Dirac operator with an electrostatic δ-interaction. Furthermore, let H_η^{nr} be the Schrödinger operator defined above. Then for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$ there is a $\kappa = \kappa(m, \lambda)$ such that

$$\left\| \big(H_\eta - (\lambda + mc^2)\big)^{-1} - \big(H_\eta^{\mathrm{nr}} - \lambda\big)^{-1} P_+ \right\| \leq \frac{\kappa}{c}.$$

J. Behrndt, P.E., M. Holzmann, V. Lotoreichik: On the spectral properties of Dirac operators with electrostatic δ-shell interactions, *J. Math. Pures at Appliquées* **111** (2018), 47–78.

A few remarks

- The convergence rate for the free Dirac operator, $\eta = 0$, is known, which allows to say that that the *result is optimal.*

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- on the other hand, for $\eta < 0$ the number of bound states of $H_\eta^{\rm nr}$ grows with the coupling strength. This yields

Proposition

For any fixed $j \in \mathbb{N}$ there is an $\eta < 0$ such that $\sharp\sigma_{\rm disc}(H_\eta) > j$ holds for all sufficiently large c.

It remains to say

Thank you for your attention!