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Distinguished self-adjoint extension for Dirac operator with potential dominated by multicenter Coulomb potentials

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Abstract. The existence and the uniqueness of the distinguished self-adjoint extension of the Dirac operator describing an electron in the field of a finite number of point charges with $Z < 137$ is proved.

In [1] we proved some general results about perturbation of non-semibounded self-adjoint operators by quadratic forms. These results were applied to obtain distinguished self-adjoint extensions for Dirac operators with singular potentials. Let H_m be the free particle Dirac operator and $V(x)$ the 4×4 symmetric matrix valued function which represents the potential. Then, one of the results in [1] is

Theorem 1. If

$$\| \| V(x) \| \| \leq v/|x|, \quad 0 \leq v < 1 \quad (1)$$

(here $\| \cdot \|$ means the usual 4×4 matrix norm and in our system of units $v = 1$ correspond to atomic number $Z = 137$) then there exists a unique self-adjoint operator H such that $f \in D(H)$ implies $f \in D(|H_m|^{1/2})$, and

$$(g, Hf) = (H_m g, f) + (Vg, f); \quad g \in D(H_m), \quad f \in D(H). \quad (2)$$

The operator H has the property

$$\sigma_{\text{ess}}(H) \subset \sigma_{\text{ess}}(H_m). \quad (3)$$

The aim of this letter is to prove the following generalization of the above result.

Theorem 1'. The conclusions of Theorem 1 remain valid if the condition (1) is replaced by

$$V(x) = \sum_{i=1}^N V_i(x); \quad \| \| V_i(x) \| \| \leq v_i/|x - x_i| \quad 0 \leq v_i < 1, \quad x_i \neq x_j, \quad N < \infty, \quad (1')$$



Remarks

1. The result contained in Theorem 1' is relevant to the bound state problem in heavy ion scattering [2].

2. Similar arguments as in the proof of Theorem 1' below, lead to the fact that the Rellich theorem [3, Th. 6.3] gives the essential self-adjointness of $H_m + V$ on $\{C_0^\infty(R^3 \setminus \{\cup_i x_i\})\}^4$ for V satisfying (1') with $0 \leq v_i \leq \frac{1}{2}$ which generalizes some results in [4].

3. Combining the proofs of Theorem 5.1 in [1] and of the Theorem 1'' one can prove a more general form of Theorem 1'. More precisely one has

Theorem 1''. *The conclusions of Theorem 1 remain valid if (1') is replaced by*

$$V(x) = V_1(x) + V_2(x)$$

where $V_1(x)$ satisfies (1') and $V_2(x)$ is nonsingular (see [1, Def. 2.1 and Def. 5.1]).

Proof of Theorem 1'. Let $d = \min_{i \neq j} |x_i - x_j|$, $\varphi(t) \in C^1([0, \infty))$ such that $\varphi(t) = 1$

for $t < d/4$, $\varphi(t) = 0$ for $t > d/3$ and $k_s(t)$ defined by

$$k_s^2(t) = \begin{cases} 1 - (m + s)t + (m^2 + s^2)t^2 & \text{for } 0 \leq t \leq (m + s)/(m^2 + s^2) \\ 1 & \text{for } t > (m + s)/(m^2 + s^2). \end{cases} \quad (4)$$

Let

$$\begin{aligned} W(x) &= V(x) - \sum_{i=1}^N \varphi(|x - x_i|) k_s^2(|x - x_i|) V_i(x) \\ &\equiv V(x) - \sum_{i=1}^N \tilde{V}_i(x) \equiv V(x) - \tilde{V}(x). \end{aligned} \quad (5)$$

From the definition of $W(x)$ it follows that

$$\sup_{x \in R^3} \|W(x)\| < \infty; \quad \sup_{x \in R^3} |x| \cdot \|W(x)\| < \infty. \quad (6)$$

Let

$$\tilde{V}(x) = \tilde{S}(x) |\tilde{V}|(x); \quad V_i(x) = S_i(x) |V_i|(x) \quad (7)$$

be the polar decompositions of $\tilde{V}(x)$ and $V_i(x)$ respectively. Using the definition $\varphi(t)$ one can see that

$$|\tilde{V}|^{1/2}(x) = \sum_{i=1}^N |V_i|^{1/2}(x); \quad \tilde{S}(x) |\tilde{V}|^{1/2}(x) = \sum_{i=1}^N S_i(x) |V_i|^{1/2}(x). \quad (8)$$

One can easily see that $W|H_m|^{-1/2}$ is compact and that \tilde{V} satisfies the conditions of Lemma 5.1 in [1] so that $[|\tilde{V}|^{1/2}(H_m - z_0)^{-1}(H_m - z)^{-1}|\tilde{V}|^{1/2}]$ (here $[\cdot]$ means the extension by continuity) is compact. Then due to the Corollary 2.1 in [1] the only thing we have to prove is that there exist $0 \leq \lambda, s < \infty$ such that

$$\| [|\tilde{V}|^{1/2}(H_m + i\lambda)^{-1}|\tilde{V}|^{1/2}] \| < 1. \quad (9)$$

Let $\Phi \in (C_0^\infty(R^3))^4$. Then from the definition of $\varphi(t)$

$$\begin{aligned} \| |\tilde{V}|^{1/2}(H_m + i\lambda)^{-1}|\tilde{V}|^{1/2}\Phi \|^2 &= \sum_{i=1}^N \| |\tilde{V}_i|^{1/2}(H_m + i\lambda)^{-1}|\tilde{V}_i|^{1/2}\Phi \|^2 \\ &\leq \sum_{i=1}^N (A_i^2 + B_i(2A_i + B_i)) \end{aligned} \quad (10)$$

where

$$A_i = \| |\tilde{V}_i|^{1/2} (H_m + i\lambda)^{-1} |\tilde{V}_i|^{1/2} \Phi \|^2, \tag{11}$$

$$B_i = \left\| \sum_{j=i}^N |\tilde{V}_j|^{1/2} (H_m + i\lambda)^{-1} |\tilde{V}_j|^{1/2} \Phi \right\|^2. \tag{12}$$

In order to prove (9) it is sufficient to show that for $\lambda = s$

$$\sum_{i=1}^N A_i^2 \leq \left(\max_i v_i^2 \right) \|\Phi\|^2, \tag{13}$$

$$\lim_{\lambda \rightarrow \infty} \left(\sup_{\Phi} B_i / \|\Phi\|^2 \right) = 0. \tag{14}$$

Now

$$\begin{aligned} A_i^2 &\leq \|k_\lambda(|\cdot - x_i|) |V_i|^{1/2} (H_m + i\lambda)^{-1} |V_i|^{1/2} k_\lambda(|\cdot - x_i|) \varphi^{1/2}(|\cdot - x_i|) \Phi\|^2 \\ &\leq v_i \|k_\lambda(|\cdot - x_i|) |\cdot - x_i|^{-1/2} (H_m + i\lambda)^{-1} |\cdot - x_i|^{-1/2} (|\cdot - x_i| |V_i|^{1/2}) \\ &\quad \cdot \varphi^{1/2}(|\cdot - x_i|) \Phi\|^2 \leq v_i^2 \|\varphi^{1/2}(|\cdot - x_i|) \Phi\|^2 \end{aligned} \tag{15}$$

In the last inequality we have used the Lemma 5.2 in [1] and the translation invariance of H_m . The inequality (13) follows from (15) and the definition of $\varphi(t)$. From the explicit form of the integral kernel of $(H_m + i\lambda)^{-1}$ (see for example [1], Section 3) one can easily see that for $|x - x_i| \leq d/3, i \neq j, \lambda > 1$

$$|((H_m + i\lambda)^{-1} |\tilde{V}_j|^{1/2} \Phi)_k(x)| \leq K \lambda^2 e^{-\lambda d} d^{-2} \|\Phi\| \tag{16}$$

so that

$$B_i \leq K' \lambda^2 e^{-d\lambda} \|\Phi\| \tag{17}$$

Then (14) is proved and the proof of the Theorem 1' is finished.

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