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Dirac operators with several Coulomb singularites

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Abstract. We study the Dirac operator with a many-center Coulomb potential with regard to the following questions: Self-adjointness, existence of a distinguished self-adjoint extension, stability of eigenvalues. In particular, we prove that also for many-center Coulomb potentials one can define a distinguished self-adjoint extension by means of a cut-off procedure. In the case of two centers we study convergence of the operator as the distance between the centers shrinks to zero.

1. Introduction

This paper deals with the operator $H = H_0 + V$, where H_0 is the free Dirac Hamiltonian and V a many-center Coulomb potential. Dirac operators for two centers have been studied extensively with regard to physical questions which arose in the field of heavy nuclei collision processes [1]. As is well-known, the Coulomb potential exhibits some mathematical peculiarities as regards self-adjointness of H. In the mathematical literature a fair amount of work has been put into studying potentials whose possible Coulomb singularity occurs at a single point. Since much less has been done in the many-center case, we felt motivated to study this case in some detail. We shall touch on the following problems.

In Section 2 we recall some important facts from the one-center case. We introduce the Birman–Schwinger kernel which will play a key role in the sequel. An important observation is that the B–S-kernel for the Coulomb potential has nonempty essential spectrum.

In Section 3 we investigate the spectrum of the operator A_E defined by (3.1). As a result we find that $D(H(\mu)) = D(H_0)$, where $H(\mu) = H_0 + \mu/|x|$ and $|\mu| < \sqrt{3}/2$ (atomic number ≤ 118), which is a recent result of Landgren and Rejto [2]. We think it makes sense to rederive this result, for there is a major difference to [2] in that we exploit the scaling (dilation) invariance of a certain operator related to A_E (see Appendix). Moreover, we get a fairly complete picture of the analyticity properties of $H(\mu)$ as a function of μ (Remark 4).

Firstly, Section 4 deals with the extension of the results of the preceding section to the many-center case. Secondly, if one or more of the centers has atomic number >118 (but <137) we construct a self-adjoint extension by removing a cut-off, thus extending Wüst's approach to several centers. As in the one center case one can completely characterize this extension by certain domain properties. Thirdly, in Theorem (4.3) we answer a question which arises naturally if of two centers one has atomic number ≤ 118 and the other >118.

Section 5 is devoted to the stability, as $R \to 0$, of the eigenvalues of $H(\mu, R) = H_0 + \mu V_R$ where $V_R(x)$ is given by (5.2). We establish norm resolvent convergence of $H(\mu, R)$ as $R \to 0$ to the 'united atom', however we encounter a problem with respect to μ. There might exist a discrete set of critical coupling constants for which our proof would break down. They are related to the possible eigenvalues of an integral kernel. Since this kernel (5.11) is genuinely two-center, we don't see how one might go about proving existence or nonexistence of these eigenvalues.

The last problem we look into concerns $\mu > 1/2$, so that the united atom has atomic number > 137. As $R \to 0$, the spectrum of $H(\mu, R)$ behaves remarkably unstable in a sense made precise in Theorem (5.8). This is a direct consequence of the spectral properties of the B–S-kernel.

Some results about the $R \to \infty$ limit will appear in [3].

2. Preliminaries

We summarize some facts about the Dirac operator with a singular potential whose only singularity is at $x = 0$. In the Hilbert space $\mathcal{H} = [L^2(\mathbb{R}^3)]^4$ let

$$H_0 = \alpha p + \beta \tag{2.1}$$

and

$$H = H_0 + V \tag{2.2}$$

where

$$\mu := \sup_{x \in \mathbb{R}^3} |xV(x)| \in (0, 1) \tag{2.3}$$

$\alpha_1, \alpha_2, \alpha_3, \alpha_4 = \beta$ are the Dirac matrices satisfying $\alpha_i \alpha_k + \alpha_k \alpha_i = 2\delta_{ik} I$ $(i, k = 1, 2, 3, 4)$. $p = -i\ (\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$. Then the following is true:

A) $H_{\min} = H \restriction C_0^\infty(\mathbb{R}^3 \backslash \{0\})$ is essentially self-adjoint if $\mu \in (0, \sqrt{3}/2)$ and in general not essentially self-adjoint for larger μ. (Ess. self-adjointness holds if $\mu = \sqrt{3}/2$ and $V(x) = \mu/|x|$).

B) If $\mu < 1$ one can single out a 'physically distinguished' self-adjoint extension (denoted by $\tilde{H}$) which is uniquely characterized either by the property

$$D(\tilde{H}) \subset D(1/\sqrt{|x|}) \tag{2.4}$$

or

$$D(\tilde{H}) \subset D(|H_0|^{1/2}) \tag{2.5}$$

Then

$$\begin{aligned} D(\tilde{H}) &= D(H_{\min}^*) \cap D(1/\sqrt{|x|}) \\ &= D(H_{\min}^*) \cap D(|H_0|^{1/2}) \end{aligned} \tag{2.6}$$

Moreover $\sigma_{\text{ess}}(\tilde{H}) = \sigma_{\text{ess}}(H_0) = \mathbb{R} \backslash (-1, 1)$. For details we refer to [4] and the references listed there. We also recall that $\tilde{H}$ is the norm resolvent limit of Hamiltonians with cut-off potentials [4], [17].

C) Let

$$R(E):=(\tilde{H}-E)^{-1},\ R_0(E)=(H_0-E)^{-1},$$
$$K_E=|V|^{1/2}\,R_0(E)V^{1/2}(V^{1/2}:=|V|^{1/2}\operatorname{sgn}V).$$

Then [4], [13]

$$R(E)=R_0(E)-R_0(E)V^{1/2}(1+K_E)^{-1}|V|^{1/2}\,R_0(E) \tag{2.7}$$

as long as -1 is not in the spectrum of K_E. For instance (2.7) holds for $E=0$ [4].

D) The Birman–Schwinger principle is valid. It says that $E\in(-1,1)$ is an eigenvalue of H with multiplicity k if and only if -1 is an eigenvalue of K_E with (geometric) multiplicity k. Since the proof by Simon [14, pp. 80–83] for Schrödinger operators carries over with little change we omit it here. We only remark that for the scale spaces we take $\mathcal{H}_{\pm1}=D(|H_0|^{\pm1/2})$ endowed with the graph norm.

E) It is illuminating and useful later on to know the spectrum of K_E if $V(x)=-\mu/|x|$, $\mu\in(0,1)$. Let $P_\Omega(A)$ denote the projection-valued measure associated with any self-adjoint operator A. Then:

(i) $\sigma(K_E)=-\sigma(K_{-E})$
(ii) $\sigma_{\mathrm{ess}}(K_E)=[-\mu,\mu]$, $E\in(-1,1)$.
(iii) $\dim P_{(\mu,\infty)}(K_E)=0$ if $E\in(-1,0]$
(vi) $0<\dim P_{(\mu,\infty)}(K_E)<\infty$ if $E\in(0,1)$.
(v) $\dim P_{(\mu,\infty)}(K_E)\to\infty$ as $E\uparrow 1$.
(vi) $\max[\sigma(K_E)]=\mu/\sqrt{1-E^2}$ if $E\in[0,1)$.

(i) was proved in [4]. (ii) will be proved in Lemma (5.5). It suffices to consider $E=0$ since K_E-K_0 is compact. (iii) Since $K_E\leqslant K_0$ if $E\in(-1,0)$ [4] we need only consider $E=0$. But $\dim P_{(\mu,\infty)}(K_0)>0$ would imply (by the Birman–Schwinger principle) that $0\in(\mathrm{H}_0-\tilde{\mu}/|x|)$ for some $\tilde{\mu}<\mu$. This is impossible for one knows (see remark below) that the lowest eigenvalue of $H_0-\mu/|x|$ is at $\sqrt{1-\mu^2}$ [7]. This yields (vi) and the first inequality in (iv). (iv) and (v) say that $\dim P_{(0,E)}$ $H_0-\mu/|x|)\to\infty$ as $E\uparrow 1$. This is well-known [7].

Remark. In proving (iii) we have tacitly assumed that in the range $\mu\in(\sqrt{3}/2,1)$ the physically distinguished extension as characterized by (2.4) (2.5) is identical with the operator considered in quantum mechanics text books, e.g. [7], which is commonly described in terms of a boundary condition at 0 (for radial two component spinors) rather than by its domain. So there arises the question of how these two approaches are linked together. We content ourselves with the remark that Weidmann's results [8] allow us to prove this equivalence.

3. Self-adjointness in the one-center problem

For the study of self-adjointness questions it is useful to have spectral information about

$$A_E:=\frac{1}{|x|}(H_0-E)^{-1},\qquad E\in\rho(H_0). \tag{3.1}$$

In particular one wants to know whether $-1 \in \rho(\mu A_E)$. If this is true for $E = \pm i$, say, it follows as in the Kato–Rellich theorem [9] that $H(\mu) = H_0 + \mu/|x| \upharpoonright D(H_0)$ is *self-adjoint*. Recently the operator A_E has been analyzed by Landgren and Rejto [2] whose results we shall rediscover. Although our methods overlap to some extent with theirs we differ by exploiting the *dilation invariance* of certain operators. The ideas of this section carry over to the many-center case. Moreover, we can say something about $H(\mu)$ as an analytic family in μ (Remark 4).

Lemma (3.1). (i) *$\sigma(A_E)$ is contained in the region enclosed by the curve $\Gamma = \{\xi_1(k) | k \in \mathbb{R}\}$ defined in* (A.6) *of the appendix with the exception of possible isolated eigenvalues of finite multiplicities outside Γ.*

(ii) *If $\operatorname{Im} E \neq 0$ then A_E has no real eigenvalues*

(iii) *If $E = 0$, A_0 has no eigenvalues outside Γ*

(*iv*) *The spectral radius of A_0 is equal to $\xi_1(0) = 2/\sqrt{3}$.*

Proof. (i) Set $E = 0$ and $A_0 = A$. Write

$$A = \chi_1 A \chi_1 + (1-\chi_1)A(1-\chi_1) + \chi_1 A(1-\chi_1) + (1-\chi_1)A\chi_1 \tag{3.2}$$

where $\chi_1(x) = 1$ if $|x| < 1$ and 0 otherwise. The second and the last term on the r.h.s. of (3.2) are compact since $(1-\chi_1)\,|x|^{-1}$ is H_0-compact. On writing $\chi_1(x) = \chi_1(2x) + (\chi_1(x) - \chi_1(2x))$ the third term is seen to be a sum of a Hilbert–Schmidt and a compact operator. The Hilbert–Schmidt property follows from the x-space representation of the integral kernel [10]. From $H_0^{-1} = (\alpha p + \beta)/(p^2+1)$ and the p^2+1-compactness of $1/|x|$ we see that the only non-compact term is

$$\chi_1 \frac{1}{|x|} \frac{\alpha p}{p^2+1} \chi_1 \tag{3.3}$$

This operator differs from

$$\tilde{A}_1 \equiv \chi_1 \frac{1}{|x|} \frac{\alpha p}{p^2} \chi_1 \tag{3.4}$$

by

$$\chi_1 \frac{1}{|x|} \frac{\alpha p}{p^2(p^2+1)} \chi_1 = \left(\chi_1 \frac{1}{|x|\,(p^2+1)}\right)\left(\frac{\alpha p}{p^2}\chi_1\right) \tag{3.5}$$

Both factors on the r.h.s. of (3.5) are compact. For the second factor this follows from the compactness of $\frac{1}{p}\chi_1$, i.e. the compactness of $\chi_1 \frac{1}{p^2}\chi_1$ which is a well known fact. Thus we are left with $\tilde{A}_1$. Introducing

$$\tilde{A}_2 \equiv (1-\chi_1)\frac{1}{|x|}\frac{\alpha p}{p^2}(1-\chi_1) \tag{3.6}$$

and

$$B \equiv \frac{1}{|x|}\frac{\alpha p}{p^2} \tag{3.7}$$

and noting that

$$\chi_1 \frac{1}{|x|} \frac{\alpha p}{p^2} (1-\chi_1)$$

is again compact

$$\left(\frac{1}{|p|} \frac{1}{|x|} \chi_1 \text{ is compact}\right),$$

we get

$$B = \tilde{A}_1 + \tilde{A}_2 + \text{compact} \tag{3.8}$$

In the appendix we prove $\sigma(B)=\Gamma$. Since in the unbounded component of the resolvent of B (i.e. outside Γ) $\|(B-z)^{-1}\| \to 0$ as $|z| \to \infty$ we can apply the analytic Fredholm theorem and conclude that any spectrum of $\tilde{A}_1+\tilde{A}_2$ must lie inside Γ with the exception of possible isolated eigenvalues of finite multiplicities outside Γ. But $\tilde{A}_1$ and $\tilde{A}_2$ have orthogonal invariant subspaces. Thus $\tilde{A}_1$ and therefore A has similar spectral properties. Using that $A_E - A$ is compact completes the proof of part (i).

(ii) Suppose $A_E f = \lambda f$ where Im $E \neq 0$, $f \neq 0$, $\lambda \neq 0$, $\lambda \in \mathbb{R}$. Since $D(H_0) \subset D(|x|^{-1})$ we conclude that $(H_0 - (\lambda\,|x|)^{-1})g = Eg$ where $g = (H_0 - E)^{-1} f$, contradicting the fact that $H_0 - (\lambda|x|)^{-1}$ is symmetric. Since Ker $A_E = \{0\}$, $\lambda = 0$ is not eigenvalue either. This proves part (ii).

(iii) Suppose $A_0 f = \lambda f$, $Im\,\lambda \neq 0$, $f \neq 0$. Then $\lambda(f, |x| f) = (f, H_0^{-1} f)$ is real, so $(f, |x| f) = 0$, i.e. $f = 0$. Thus there are no complex eigenvalues. Suppose now Im $\lambda = 0$. Then $g = (1/\sqrt{|x|}) H_0^{-1} f$ obeys $(1/\sqrt{|x|}) H_0^{-1} (1/\sqrt{|x|}) g = \lambda g$ Hence $|\lambda| \leq 1 < \xi_1(0) = 2/\sqrt{3}$ using property (vi) of Sect. 2.

(iv) Follows from (iii) noting that $|\xi_1(k)| \leq \xi_1(0)$, $k \in \mathbb{R}$.

Remarks. 1) Lemma (3.1) implies self-adjointness of $H(\mu)$ when $|\mu| < \sqrt{3}/2$.

2) In the many-center case we shall replace A_E by $\chi_\delta A_E \chi_\delta$ $(\delta > 0)$ where $\chi_\delta(x) = 1$ if $|x| < \delta$ and 0 otherwise. Lemma (3.1) is still true with obvious modifications of the proof.

3) (ii) holds (by the same proof) for general H_0-bounded potentials $V(x)$.

4) We invite the reader to draw a picture of Γ and of $\Gamma^{-1} = \{z \in \mathbb{C} \mid 1/z \in \Gamma\}$. $H(\mu)$ is closed for all μ outside Γ^{-1} and forms a holomorphic family of type A [9, p. 375]. One observes that the half-line $t \exp(i\varphi)$, $t \in (0, \infty)$ intersects Γ^{-1} twice (respectively never) if $|\varphi| < \alpha$, $|\pi - \varphi| < \alpha$, $\varphi \neq 0$, π, where α is given by $\tan(2\alpha) = \frac{1}{2}$(respectively $|\varphi| > \alpha$, $\alpha < |\varphi| < \pi - \alpha$). The half-lines $\varphi = 0$ or π and $t > \sqrt{3}/2$ lie inside Γ^{-1}. This leads to the interesting conclusion that no matter how small $\varphi(\varphi \neq 0)$ is, $H(\mu)$ is closed for sufficiently large $|\mu|$, where $\mu = |\mu| \exp(i\varphi)$. The curve Γ^{-1} is, however, *not* a border line as regards the analyticity of the *resolvent* of $H(\mu)$. Using (2.7) on concludes that $H(\mu)^{-1}$ can be analytically continued to the interior of Γ^{-1}. Denoting this continuation by $\tilde{H}(\mu)^{-1}$ one verifies that $\tilde{H}(\mu)$ is a closed extension of $H(\mu)$ and $D(\tilde{H}(\mu)) \subset D(1/\sqrt{|x|})$ and $D(\tilde{H}(\mu)) \subset D(|H_0|^{1/2})$. $\tilde{H}(\mu)^{-1}$ is analytic in $\mathbb{C} \setminus \{\mu \mid \mu \in \mathbb{R}, |\mu| \geq 1\}$. This generalizes the result of Kato [9, p. 308].

5) Using the relationship between solutions of $H(\mu)^* f = if$ and of $A_i^* f = -f$ we can show that the interior of Γ belongs to the residual spectrum of A_i. Γ itself

forms the continuous spectrum. Then one also recognizes that $\Gamma^{-1} = \{\mu \mid \operatorname{Re}\sqrt{1-\mu^2} = \frac{1}{2}\}$ which is related to the square-integrability of f near 0, since $f \approx |x|^{-1-\sqrt{1-\mu^2}}$ near 0.

4. Self-adjoint extensions in the many-center case

4.1 *Self-adjointness*

In this section we shall prove

Theorem (4.1). *Let $\mu_i \in \mathbb{R}$, $|\mu_i| < \sqrt{3}/2$ $(i = 1 \cdots N)$, $a_i \in \mathbb{R}^3$, $a_i \neq a_j$ $(i \neq j)$ be given. Let*

$$V(x) = \sum_{i=1}^{N} \frac{\mu_i}{|x - a_i|}$$

Then $H = (H_0 + V) \restriction D(H_0)$ is self-adjoint.

Remarks. 1) If one is willing to settle for essential self-adjointness on $[C_0^\infty(\mathbb{R}^3)]^4$ there is an elegant method due to Chernoff [11].

2) The case $|\mu_i| < \frac{1}{2}$ has been treated in a remark by Nenciu [12].

3) Theorem (4.1) shows that H is essentially self-adjoint on any core for H_0, e.g. on $C_0^\infty\left(\mathbb{R}^3 \Big\backslash \left\{\bigcup_{i=1}^{n} a_i\right\}\right)$.

Proof. Choose δ such that $0 < \delta < \frac{1}{2} \min_{i \neq j} |a_i - a_j|$. Then

$$V(H_0 - E)^{-1} = \sum_{i=1}^{N} \mu_i \frac{\chi_\delta(x - a_i)}{|x - a_i|} (H_0 - E)^{-1} \chi_\delta(x - a_i) + \text{compact} \tag{4.1}$$

From Remark 2 to Lemma (3.1) and the assumptions on μ_i we obtain

$$-1 \in \rho\left(\mu_i \frac{\chi_\delta(x - a_i)}{|x - a_i|} (H_0 - E)^{-1} \chi_\delta(x - a_i)\right) \tag{4.2}$$

for every i.

Consequently, (4.2) is true with the r.h.s. replaced by the sum over i, for this sum can be viewed as a *direct* sum. Assuming $\operatorname{Im} E \neq 0$ and using Remark 3 to Lemma (3.1) we conclude that $V(H_0 - E)^{-1}$ has no real eigenvalues. So

$$-1 \in \rho(V(H_0 - E)^{-1}), \tag{4.3}$$

proving the self-adjointness of H.

4.2 *The distinguished extension*

In this section let

$$V(x) = -\sum_{i=1}^{N} \frac{\mu_i}{|x - a_i|} \tag{4.4}$$

where $0 < \mu_i < 1$ $(a_i \neq a_j, i \neq j)$.

We consider

$$H \equiv H_0 + V \upharpoonright C_0^\infty\left(\mathbb{R}^3 \setminus \left\{\bigcup_{i=1}^N a_i\right\}\right) \tag{4.5}$$

and try to construct a self-adjoint extension which is acceptable for physics. In the author's opinion, the most convincing way to do this is by means of cut-off potentials. We shall prove that as $n \to \infty$

$$H_n = H_0 + V_n, \tag{4.6}$$

where $V_n(x) = \max(-n, V(x))$, converges in norm resolvent sense to a self-adjoint operator $\tilde{H}$, and it seems reasonable to consider $\tilde{H}$ as relevant for physics. As we shall see, $\tilde{H}$ has many other properties which are desirable and which we accept graciously!

In Theorem (4.2) we shall prove that $\tilde{H}$ can indeed be constructed by the method of cut-off potentials, thereby extending Wüst's results [6] about the one center case to several centers. To avoid some technical complications we have assumed that all $\mu_i > 0$. Of course, only notational changes would be needed to cover the case where all $\mu_i < 0$, however, if the μ_i take both signs more work is necessary (see [17] for one center). In Wüst's work a critical ingredient is that H_n has a gap in the spectrum whose width is independent of n. In the course of the proof of Theorem (4.1) we shall see that this is also true in case of several centers.

A Hamiltonian with potential (4.4) has been constructed previously by Nenciu [12], using as a criterion the requirement $D(\tilde{H}) \subset D(|H_0|^{1/2})$. We shall see that our extension is the same. Finally, in Theorem (4.3), we consider a special case of two centers, namely

$$H = H_0 + V + W$$

where V, W are Coulomb potentials such that $H_0 + V$ is *not* essentially self-adjoint while $H_0 + W$ is self-adjoint. We shall prove that

$$\tilde{H} = (H_0 + V)^\sim + W,$$

meaning one can get $\tilde{H}$ by adding one center after the other. Moreover, it will follow that H is not essentially self-adjoint.

Theorem (4.2). (i) *$\tilde{H}$ = norm resolvent* lim H_n $(n \to \infty)$ *exists and is a self-adjoint extension of H.*
(ii) $D(\tilde{H}) = D(H^*) \cap D(|V|^{1/2})$
(iii) $\sigma_{\text{ess}}(\tilde{H}) = \sigma_{\text{ess}}(H_0)$

The proof of this theorem depends heavily on

Lemma (4.3). *Let $K_{E,n} = |V_n|^{1/2}(H_0 - E)^{-1}|V_n|^{1/2}$. Then we can find $E \in (-1, 1)$ and a constant C such that for sufficiently large n*

$$\|(1 - K_{E,n})^{-1}\| \leq C \tag{4.7}$$

Proof. Following an argument of Nenciu [13] we note that $1 \in \rho(K_{E,n})$ for all $E \in \rho(H_0)$ with the possible exception of a discrete set provided we can find one value of E where this holds. Pick $E = is$, $s \in \mathbb{R}$, and use

$$(H_0 - E)^{-1} = \frac{\alpha p + \beta + E}{p^2 + 1 - E^2} \tag{4.8}$$

Then

$$\operatorname{Im}(f, K_{is,n} f) \neq 0 \tag{4.9}$$

if $f \neq 0$ and $s \neq 0$. This implies that 1 cannot be eigenvalue of $K_{is,n}$. We want to show that 1 does not belong to the spectrum at all. Let $D_i = \chi_\delta(x - a_i)$, $D = \sum D_i$. Multiply $K_{E,n}$ from both sides by $[D + (1-D)]$ and expand.

Firstly, $(1-D)K_{E,n}(1-D)$ is compact and independent of n (for n large enough). Secondly, the terms $D_i K_{E,n}(1-D)$ (or D and D_i switched) are compact and have norm limits as $n \to \infty$. To this end write

$$\chi_\delta(x - a_i)\,|V_n|^{1/2}(H_0 - E)^{-1} = \chi_\delta(x - a_i)|x - a_i|^{1/2}\,|V_n|^{1/2}) \times (|x - a_i|^{-1/2}(H_0 - E)^{-1}) \tag{4.10}$$

and note that the r.h.s. is of the form $A_n B$ where $A_n \to A$ strongly and B is compact. Hence $A_n B \to AB$ in norm. Thirdly, $D_i K_{E,\,n} D_j$ $(i \neq j)$ is Hilbert–Schmidt and tends to a limit in Hilbert–Schmidt norm (consider the kernel in x-space [10]). Fourthly, terms of the type $D_i K_{E,n} D_i$ are equal to

$$(\chi_\delta(x - a_i)|V_n|^{1/2}\,|x - a_i|^{1/2})\frac{1}{|x - a_i|^{1/2}}(H_0 - E)^{-1} \times \frac{1}{|x - a_i|^{1/2}}(|x - a_i|^{1/2}\,|V_n|^{1/2}\chi_\delta(x - a_i)) \tag{4.11}$$

Now we choose δ so small that for all $i = 1 \cdots N$ the factors in parentheses have norm smaller than $1 - \delta_1$ with some $\delta_1 > 0$. This is possible since $|\mu_i| < 1$. Since $\| |x|^{-1/2} H_0^{-1} |x|^{-1/2} \| \leq 1$ [4], and H_0 is translation invariant we see that at $E = 0$ the norm of (4.11) is less than $1 - \delta_1$ uniformly in n. This implies that for $E \in \rho(H_0)$

$$\sigma_{\text{ess}}(K_{E,n}) \subset [-1 + \delta_1, \quad 1 - \delta_1] \tag{4.12}$$

(using that $K_{E,n} - K_{0,n}$ is compact) which, along with (4.9), proves that $1 \in \rho(K_{E,n})$ if $E = is$, $s \neq 0$. Thus $1 \in \rho(K_{E,n})$ with the possible exception of a discrete set on $(-1, 1)$.

All these facts hold for the limiting operators $(n = \infty)$ as well. Consequently, we can pick $E \in (-1, 1)$ such that $1 \in \rho(K_{E,\infty})$. Then

$$K_{E,n} = K_{E,n}^{(1)} + K_{E,n}^{(2)} \tag{4.13}$$

$$= K_{0,n}^{(1)} + K_{E,n}^{(1)} - K_{0,n}^{(1)} + K_{E,n}^{(2)} \tag{4.14}$$

$$= K_{0,n}^{(1)} + B_n \tag{4.15}$$

where $K_{E,n}^{(1)}$ is (4.11) summed over all i and $K_{E,n}^{(2)}$ comprises the rest which is compact. As $n \to \infty$, $K_{E,n}^{(1)} - K_{0,n}^{(1)}$ and $K_{E,n}^{(2)}$ have norm limits. For the latter this has been proved above. As to the former note that

$$K_{E,n}^{(1)} - K_{0,n}^{(1)} = E|V_n|^{1/2}(H_0 - E)^{-1}H_0^{-1}|V_n|^{1/2} \tag{4.16}$$

so that we can apply an argument similar to that in (4.10). Now $1 \in \rho(K_{E,n})$ if and only if

$$1 \in \rho((1 - K_{0,n}^{(1)})^{-1}B_n) \tag{4.17}$$

by (4.15) and since $\|(1 - K_{0,n}^{(1)})^{-1}\| < 1/\delta_1$. Now $(1 - K_{0,n}^{(1)})^{-1}$ has a strong limit whereas B_n is compact and has a norm limit. Hence the product has a norm limit. Therefore, knowing (4.17) for $n = \infty$ yields

$$\|(1 - (1 - K_{0,n}^{(1)})^{-1}B_n)^{-1}\| \leq \tilde{C} \tag{4.18}$$

for some constant $\tilde{C}$ and large enough n. Since

$$(1 - K_{E,n})^{-1} = (1 - K_{0,n}^{(1)})^{-1}B_n)^{-1}(1 - K_{0,n}^{(1)})^{-1} \tag{4.19}$$

(4.7) follows from (4.18) with $C = \tilde{C}/\delta_1$.

Proof of Theorem (4.2). (i) Let E be as for (4.7). Then, as $n \to \infty$

$$(H_n - E)^{-1} = (H_0 - E)^{-1} + (H_0 - E)^{-1}\sqrt{|V_n|}(1 - K_{E,n})^{-1}\sqrt{|V_n|}(H_0 - E)^{-1} \tag{4.20}$$

tends in norm to a limiting operator (with V_n replaced by V), for $(H_0 - E)^{-1}\sqrt{|V_n|}$ is compact and normconvergent and $(1 - K_{E,n})^{-1}$ is strongly convergent. To prove that the limit of $(H_n - E)^{-1}$ is the resolvent of a self-adjoint extension of H one can either follow the method of Nenciu [13] or Wüst [5]. Since we are heading towards a proof of (ii) it is appropriate to follow Wüst. Note that $\|(H_n - E)^{-1}\| \leq C$ implies $\|(H_n - E)f\| \geq C^{-1}\|f\|$, $f \in D(H_n) = D(H_0)$, i.e. there exists for all large enough n a gap of constant width in the spectrum of H_n near E. We can identify the limit of $(H_n - E)^{-1}$ with $(H_g - E)^{-1}$ where H_g denotes the strong graph limit of H_n (cf. Prop. 2 of [5]). $H_g = \tilde{H}$ is a self-adjoint extension of H proving (i).

(ii) Note that $D(\tilde{H}) \subset D(H^*)$ by general theory and $D(\tilde{H}) \subset D(|V|^{1/2})$ by (4.20) and the uniform boundedness of $|V|^{1/2}(H_0 - E)^{-1}|V_n|^{1/2}$, which follows from $|V_n| \leq |V|$. Thus $D(H) \subset D(H^*) \cap D(|V|^{1/2})$. To prove the converse we follow Wüst [6, p. 97,1. Step]. Since there is one important change we give the argument. Pick $u \in D(\tilde{H})$. Let $u_n \in D(H_n)$ be such that $u_n \to u$, $H_n u_n \to \tilde{H}u$. Let $u_n^{(k)} \to D(H)$ obey $u_n^{(k)} \to u_n$, $H_n u_n^{(k)} \to H_n u_n$ as $k \to \infty$ using that $D(H)$ is a core for H_n. Pick $f \in D(H^*) \cap D(|V|^{1/2})$. Then

$$(H^*f, u) - (f, Hu) = \lim_{n \to \infty} \lim_{k \to \infty} (f, (V - V_n)u_n^{(k)}) \tag{4.21}$$

By the Schwarz inequality

$$\begin{aligned} |(f, (V - V_n)u_n^{(k)})| &= |(f, (V - V_n)|V|^{-1/2}\ |V|^{1/2}u_n^{(k)})| \\ &\leq \||V|^{-1/2}(V - V_n)f\|\ \|\ |V|^{1/2}u_n^{(k)}\| \end{aligned} \tag{4.22}$$

Now

$$\begin{aligned} \||V|^{1/2}u_n^{(k)}\| &= \||V|^{1/2}(H_n - i)^{-1}(H_n - i)u_n^{(k)}\| \\ &\leq C\|(H_n u_n^{(k)} + u_n^{(k)})\| \end{aligned} \tag{4.23}$$

where $C=\sup_n \| |V|^{1/2}(H_n-i)^{-1}\|$ is finite by (4.20), noting that

$$\| |V|^{1/2}(H_0-i)^{-1}|V_n|^{1/2}\| = \| |V|^{1/2}(H_0-i)^{-1}|V|^{1/2}\,|V|^{-1/2}|V_n|^{1/2}\| \leq \| |V|^{1/2}(H_0-i)^{-1}|V|^{1/2}\| \tag{4.24}$$

The last inequality in (4.23) follows from the graph convergence. Since $f\in D(|V|^{1/2})$, $\| |V|^{-1/2}(V-V_n)f\|\to 0$ as $n\to\infty$. Hence (4.21) is zero, proving that $f\in D(H^*)=D(H)$. This completes the proof of part (ii).

(iii) $(H-E)^{-1}-(H_0-E)^{-1}$ is compact on account of (4.20), proving the claim.

Remarks. 1) We differ from Wüst's proof by using (4.20), which immediately leads to (4.24).

2) (4.20) shows that $D(\tilde{H})\subset D(|H_0|^{1/2})$, proving equality of $\tilde{H}$ and Nenciu's extension.

3) As in the one-center case, $\tilde{H}$ is uniquely characterized by demanding $D(\tilde{H})\subset D(|V|^{1/2})$.

Now we turn to the problem of two centers mentioned at the beginning of this section.

Let $V(x)=-\mu/|x|$, $\mu\in(\sqrt{3}/2,1)$ and $W(x)=-\sigma/|x-a|$, $\sigma\in(0,\sqrt{3}/2)$, $a\neq 0$. Then we can construct $\tilde{H}=(H_0+V+W)^{\tilde{}}$ or $(H_0+V)^{\tilde{}}+W$ (anticipating that $D(W)\supset D(H_0+V)^{\tilde{}}$.). We shall prove

Theorem (4.3). (i) $(H_0+V)^{\tilde{}}+W=\tilde{H}$
(ii) $\bar{H}=\overline{H_0+V+W}$ ($\bar{}$ means closure)

Remark. Since $D(\overline{H_0+V})\neq D((H_0+V)^{\tilde{}})$ we see that H (see (4.5)) is *not* essentially self-adjoint.

We need

Lemma (4.4). (i) $D((H_0+V)^*)=D(H^*)$
(ii) $D(H)\subset D(H^*)\subset D(W)$
(iii) $D((H_0+V)^{\tilde{}})\subset D((H_0+V)^*)\subset D(W)$

Proof of Lemma (4.4). (i) Suppose $f\in D((H_0+V)^*)$. Choose $\varphi\in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, $\varphi\equiv 1$ for $|x-a|<|a|/2$ and $\varphi=\bar{\varphi}$.

Claim: φf and $(1-\varphi)f\in D(H^*)$.

Pick $g\in D(H)=[C_0^\infty(\mathbb{R}^3\backslash\{0,a\})]^4$ and set $\tilde{\varphi}=1-\varphi$. Then

$$(\tilde{\varphi}f, Hg)=(f,\tilde{\varphi}Hg)=(f,H\tilde{\varphi}g)-(\bar{g}f,(\alpha p)\tilde{\varphi}) \tag{4.25}$$

$$=(f,(H_0+V)\tilde{\varphi}g)+(F,W\tilde{\varphi}g)-(\bar{g}f,(\alpha p)\tilde{\varphi}) \tag{4.26}$$

$$=((H_0+V)^*f,\tilde{\varphi}g)+(f,W\tilde{\varphi}g)-(\bar{g}f,(\alpha p)\tilde{\varphi}) \tag{4.27}$$

Thus

$$|(\tilde{\varphi}f, Hg)|\leq C\|g\| \tag{4.28}$$

for $\|W\tilde{\varphi}\|_\infty<\infty$, $\|(\alpha p)\tilde{\varphi}\|_\infty<\infty$.

Hence

$$\tilde{\varphi}f\in D(H^*) \tag{4.29}$$

Likewise,

$$|(\varphi f, H_0 g)| = |(f, (H_0+V)\varphi g) - (\bar{g}f, (\alpha p)\varphi) - (f, V\varphi g)| \\ \leq \tilde{C}\,\|g\| \tag{4.30}$$

Since $D(H)$ is a core for H_0 we see that $\varphi f \in D(H_0) \subset D(\bar{H}) \subset D(H^*)$(the second inclusion is a consequence of H_0-boundedness of V and W). Thus $\varphi f \in D(H^*)$, so $f \in D(H^*)$(by (4.29)), proving $D((H_0+V)^*) \subset D(H^*)$.

Conversely, suppose $f \in D(H^*)$. Then $\tilde{\varphi} f \in D((H_0+V)^*)$ by combining (4.25) and (4.26). Now $(\varphi f,(H_0+W)g) = (f,(H_0+W)g\varphi) - (f\bar{g},(\alpha p)\varphi) = (f, Hg\varphi) - (f, Vg\varphi) - (f\bar{g}, (\alpha p)\varphi)$ showing that $\varphi f \in D(H_0+W)$. But $D(H_0+W) = D(H_0)$, so $\varphi f \in D(H_0) \in D((H_0+V)^*)$. Thus $f \in D((H_0+V)^*)$, proving (i).

(ii) Let $f \in D(H^*)$. By the above, $\varphi f \in D(H_0) \subset D(W)$. But $\tilde{\varphi} f \subset D(W)$ for any f. Hence $D(W) \supset D(H^*) \supset D(\tilde{H})$, proving (ii).

(iii) The first inclusion is standard, the second follows immediately from (i) and (ii).

Proof of Theorem (4.3).

$$\text{(i)}\ D(\tilde{H}) = D(H^*) \cap D(|V|^{1/2}) \cap D(|W|^{1/2}) = D(H^*) \cap D(|V|^{1/2}) \\ = D((H_0+V)^*) \cap D(|V|^{1/2}) = D((H_0+V)^{\tilde{}}) \\ = D((H_0+V)^{\tilde{}} + W),$$

proving (i). The first equality is (ii) of Theorem (4.2). The second follows from Lemma (4.4)(ii) and $D(|W|) \subset D(|W|^{1/2})$. Then we use Lemma (4.4)(i), Theorem (4.2)(ii) and Lemma (4.4)(iii).

(ii) By Lemma (4.4)(iii) W is $(H_0+V)^{\tilde{}}$-bounded. This implies that Wf_n is Cauchy whenever $f_n \in D(H_0+V)$ is Cauchy $(D(H_0+V) = [C_0^\infty(\mathbb{R}^3 \setminus \{0\})]^4)$. Thus $(H_0+V+W)f_n$ converges, proving $\bar{H} \subset H_0+V+W$. By Lemma (4.4)(ii) W is $\tilde{H}$-bounded. Therefore $\bar{H} \supset H_0+V+W$.

5. Stability of eigenvalues for two centers

5.1 *The problem*

Consider the Hamiltonian

$$H(\mu, R) := H_0 - \mu V_R, \qquad \mu \in (0, \tfrac{1}{2}) \tag{5.1}$$

where

$$V_R = \frac{1}{|x|} + \frac{1}{|x-R|}, \qquad R = (|R|, 0, 0) \tag{5.2}$$

For simplicity we restrict ourselves to the case of two equal, negatively charged nuclei. If $R \neq 0$ we mean by (5.1) the self-adjoint operator defined on $D(H_0)$(cf. Sect. 4). If $R = 0$, the correct extension to be taken will be the physically distinguished one (cf. Sect. 2B). We set $H(\mu, 0) = H(2\mu)$.

The main question we try to answer in this section is about the convergence of $H(\mu, R)$ toward $H(2\mu)$ as $R \to 0$. In Theorem (5.7) we shall prove norm resolvent convergence but, unfortunately, we have to exclude a discrete set of

μ-values. We are able to identify these critical coupling constants via the eigenvalues of an integral kernel (5.11). It is, however, entirely conceivable to us that these eigenvalues are absent, but we have been unable to prove this.

For noncritical coupling constants stability of eigenvalues (cf. Kato [9]) is a direct consequence of norm resolvent convergence.

In the context of heavy nuclei collision processes, perturbation calculations for the energies have been carried out by Greiner and Müller [1] for small (and large) R. This was done in the scheme of the 'united atom approximation', familiar from nonrelativistic problems. We do not attempt to justify the applicability of this method in the Dirac case. However it is instructive to think a bit about some problems related to this method. Write

$$H(\mu, R)=H(2\mu)+\mu W_R, \qquad W_R(x)=\frac{2}{|x|}-\frac{1}{\left|x-\dfrac{R}{2}\right|}-\frac{1}{\left|x+\dfrac{R}{2}\right|}. \tag{5.3}$$

If H_0 were the Laplacian it would be perfectly possible to estimate

$$|W_R(x)|\leqslant \text{const.}\ |R|^\delta\left(\frac{2}{|x|^{1+\delta}}+\frac{1}{\left|x-\dfrac{R}{2}\right|^{1+\delta}}+\frac{1}{\left|x+\dfrac{R}{2}\right|^{1+\delta}}\right) \tag{5.4}$$

where $\delta\in(0, 1)$. In the Dirac case, however, a potential like $|x|^{-(1+\delta)}$ is certainly not what we desire. Furthermore, it is *not* true that $\|W_R(H(2\mu)-i)^{-1}\|\to 0$ as $R\to 0$ (assuming $0\leqslant 2\mu<\sqrt{3}/2$ so that $D(H(2\mu))=D(H_0)\subset D(W_R)$). Since $1\in \rho((2\mu/|x|)(H_0-i)^{-1})$ it suffices to show that $\|W_R(H_0-i)^{-1}\|\nrightarrow 0$ as $R\to 0$. By a scale transformation (using (4.8)) $W_R(H_0-i)^{-1}$ is unitarily equivalent to $W_{\hat R}(\alpha p+\beta|R|+i|R|/p^2+2R^2)$ where $\hat R=(1, 0, 0)$. As $R\to 0$, this operator tends strongly to $W_{\hat R}(\alpha p/p^2)\neq 0$. Therefore $\|W_R(H_0-i)^{-1}\|\nrightarrow 0$, proving our claim.

Next we first prove norm resolvent convergence for $\mu<1/\pi$ (Theorem (5.3)) and subsequently extend this result to larger μ. It is in the range $[1/\pi, 1)$ where the possibility of critical coupling constants arises.

5.2 $\mu<1/\pi$

We need two lemmas:

Lemma (5.1). $\|\sqrt{V_R}H_0^{-1}\sqrt{V_R}\|\leqslant\pi$ for all R.

Proof.

$$\|\sqrt{V_R}H_0^{-1}\sqrt{V_R}\|\leqslant\|\sqrt{V_R}\,|H_0|^{-1}\sqrt{V_R}\|=\||H_0|^{-1/2}V_R\,|H_0|^{-1/2}\|$$
$$=\left\|\frac{1}{(p^2+1)^{1/4}}V_R\frac{1}{(p^2+1)^{1/4}}\right\|\leqslant 2\left\|\frac{1}{(p^2+1)^{1/4}}\frac{1}{|x|}\frac{1}{(p^2+1)^{1/4}}\right\|\leqslant\pi$$

using [9, p. 307].

Remark. Only the first step is an inequality. Steps four and five are in fact equalities due to a result of Herbst [16], along with a scaling argument.

Lemma (5.2). $V_R^{1/2}H_0^{-1} \to \sqrt{\dfrac{2}{|x|}}\,H_0^{-1}$ *in norm as* $R \to 0$.

Proof. By a scale transformation it is equivalent to show that

$$|R|^{1/2}\left(W(x)\frac{1}{|p|}\right)\left(\frac{|p|\,(\alpha p+|R|\,\beta)}{p^2+R^2}\right)$$

tends to zero in norm as $R \to 0$, where $W(x) = V_R^{1/2} - \sqrt{2/|x|}$. The last factor has norm 1 and $W(x)/|p|$ is bounded, since $W(x) = 0(|x|^{-3/2})$ at infinity and the singularities are less severe than Coulombic.

Theorem (5.3). *Suppose* $0 < \mu < 1/\pi$. *Then* $H(\mu, R) \to H(2\mu)$ *in norm resolvent sense as* $R \to 0$.

Proof. In (4.20) replace V_n by V_R and $K_{E,n}$ by $K_R(E) = \mu V_R^{1/2}(H_0 - E)^{-1}V_R^{1/2}$. Choose $E = 0$ and note that $K_R(0) \to K_0(0)$ strongly as $R \to 0$, whereas $H_0^{-1}V_R^{1/2} \to H_0^{-1}V_0^{1/2}$, $V_R^{1/2}H_0^{-1} \to V_0^{1/2}H_0^{-1}$ in norm by Lemma (5.2). Lemma (5.1) ensures that $((1-K_R(0))^{-1} \to (1-K_0(0))^{-1}$ strongly, so that we can use the compactness of $V_R^{1/2}H_0^{-1}$ to conclude that the second term on the r.h.s. of (4.20) converges in norm as $R \to 0$.

5.3 $1/\pi < \mu < 1$

The problem is to find a uniform bound on $\|(1-K_R(E))^{-1}\|$ for R small. That means we need to know how the spectrum of the Birman–Schwinges kernel varies as a function of R. Although, we know everthing when $R = 0$, we are seriously hampered by the fact that the Birman–Schwinger kernel only converges *strongly* as $R \downarrow 0$.

It turns out to be advantageous to study the limit $E \downarrow -1$. However in order for this limit to exist we need a cut-off defined as

$$V_{R,\sigma} \equiv V_R \cdot \chi_\sigma \qquad (|R| < \sigma) \tag{5.5}$$

Later on we will jump from $E = -1$ to $E = 0$ and remove the cut-off. Note that (5.5) cuts off the superposed potentials. One could also cut off each individual potential and then superpose them. The difference is a boundary term which could be handled as well. Our choice here leads to some simplifications. On setting $W = V_{R,\sigma}^{1/2}$ we claim that

Lemma (5.4)

$$W(H_0 - E)^{-1}W \to W\,\frac{\alpha p}{p^2}\,W + (\beta - 1)W\frac{1}{p^2}\,W \tag{5.6}$$

in norm *as* $E \downarrow -1$.

Proof. Starting off from (4.8) we remark that the second term on the r.h.s. of (5.6) is the limit, as $E \downarrow -1$, of $W[(\beta + E)/(p^2 + 1 - E^2)]W$. Convergence holds in norm, since W has compact support and one can easily write down the x-space kernel of $1/(p^2+1-E^2)$. So we need only show that

$$W\frac{\alpha p}{p^2+1-E^2}W \to W\frac{\alpha p}{p^2}W \tag{5.7}$$

in norm as $E\downarrow -1$. We observe that the difference of these two operators is

$$-\varepsilon W\frac{\alpha p}{p^2(p^2+\varepsilon)}W, \qquad \varepsilon := 1-E^2, \tag{5.8}$$

whose norm is bounded by that of

$$\varepsilon W\frac{1}{p(p^2+\varepsilon)}W \tag{5.9}$$

Now use $p^2+\varepsilon \geqslant 2|p|\sqrt{\varepsilon}$ to recognize that the norm of (5.9) is bounded by $C\cdot\sqrt{\varepsilon}$. This proves Lemma (5.4).

Lemma (5.5). (i) $\sigma_{\text{ess}}\left(\frac{\chi_\sigma}{\sqrt{|x|}}\frac{\alpha p}{p^2}\frac{\chi_\sigma}{\sqrt{|x|}}\right) = [-1, 1], \qquad 0<\sigma\leqslant\infty.$

(ii) $\sigma_{\text{ess}}\left(V_{R,\sigma}^{1/2}\frac{\alpha p}{p^2}V_{R,\sigma}^{1/2}\right) = [-1, 1], \qquad 0<\sigma<\infty,$

$R\neq 0, \quad \sigma>|R|.$

(iii) $\sigma_{\text{ess}}\left(\frac{\chi_\sigma}{\sqrt{|x|}}H_0^{-1}\frac{\chi_\sigma}{\sqrt{|x|}}\right) = [-1, 1], \qquad 0<\sigma\leqslant\infty.$

(iv) $\sigma_{\text{ess}}(V_{R,\sigma}^{1/2}H_0^{-1}V_{R,\sigma}^{1/2}) = [-1, 1], \qquad 0<\sigma\leqslant\infty,$

$R\neq 0, \quad \sigma>|R|.$

But

(v) $\sigma_{\text{ess}}\left(V_R^{1/2}\frac{\alpha p}{p^2}V_R^{1/2}\right) = [-2, 2](!)$ *all* R.

Proof. (i) Note that any change in σ can be compensated for by a suitable scale transformation. As $\sigma\to\infty$, the strong limit is the operator studied in the Appendix, part b). Applying [18, Thm. VIII 24] and (A.12) yields the result.

(ii) Follows from (i) by 'localisation' as in Sect. 4.1.

(iii) For every σ the operator has norm $\leqslant 1$ [4]. Moreover, the operator is unitarily equivalent to

$$\frac{\chi_{\sigma/\lambda}}{\sqrt{|x|}}\frac{\alpha p+\lambda\beta}{p^2+\lambda^2}\frac{\chi_{\sigma/\lambda}}{\sqrt{|x|}}$$

where $\lambda>0$ is arbitrary and σ is fixed. Let $\lambda\downarrow 0$ and follow the argument in (i).

(iv) Follows from the preceding result.

(v) By scaling, operators with different R are unitarily equivalent. As $R\to 0$, the operator converges strongly to twice the operator of (i), thus the essential spectrum contains $[-2, 2]$. To see that, in fact, the essential spectrum cannot be larger than $[-2, 2]$, multiply the operator on both sides by $\chi_N+(1-\chi_N)$ and expand. The $\chi_N \cdots \chi_N$-term gives rise to essential spectrum $[-1, 1]$ (assuming $N>|R|$). The cross terms are compact. However, the term $(1-\chi_N)\cdots(1-\chi_N)$ gives rise to essential spectrum $[-2, 2]$. To any given $\varepsilon>0$ we can find N_0 such that this term has norm $\leqslant 2+\varepsilon$ when $N\geqslant N_0$ using that $V_R(x)\sim 2/|x|$ for large $|x|$. The two noncompact terms being orthogonal implies (v).

For any $\lambda>0$ let $(U_\lambda f)(x)=\lambda^{3/2}\ f(\lambda x)$. Denote the r.h.s. of (5.6) by $W_{R,\sigma}(H_0+1)^{-1}W_{R,\sigma}$ where now $W_{R,\sigma}=V_{R,\sigma}^{1/2}$. Let $W_{\hat{R}}=V_{\hat{R}}^{1/2}(\sigma=\infty)$. The following lemma is crucial.

Lemma (5.6)

$$P_{(a,\infty)}(U_{|R|}W_{R,\sigma}(H_0+1)^{-1}W_{R,\sigma}U^*_{|R|})\to P_{(a,\infty)}\left(W_{\hat{R}}\frac{\alpha p}{p^2}W_{\hat{R}}\right)$$

in norm *as* $R\to 0$, *for any* $a>2$.

Remark. By Lemma (5.5) and the compactness of the second term on the r.h.s. of (5.6), the spectral projections in Lemma (5.6) are finite dimensional.

Proof. From (5.6) we obtain

$$U_{|R|}W_{R,\sigma}(H_0+1)^{-1}W_{R,\sigma}U^*_{|R|}=W_{\hat{R},\sigma/|R|}\frac{\alpha p}{p^2}W_{\hat{R},\sigma/|R|}+|R|(\beta-1)W_{\hat{R},\sigma/|R|}\frac{1}{p^2}W_{\hat{R},\sigma/|R|} \tag{5.10}$$

We remark that the first term on the r.h.s. is of the form QAQ where Q is a projection (multiplication by $\chi_{\sigma/|R|}$) and $A=W_{\hat{R}}\dfrac{\alpha p}{p^2}W_{\hat{R}}$. Then one knows that dim $P_{(a,\infty)}(QAQ)\leqslant\dim P_{(a,\infty)}(A)$. To see this note that $(QAQ)_+\leqslant QA_+Q$ where the subscript $+$ refers to the positive spectral part. Now $\sigma(QA_+Q)\cap(a,\infty)=\sigma(A_+^{1/2}QA_+^{1/2})\cap(a,\infty)$, since BC is isospectral [15] to CB for any two bounded operators B, C. But $A_+^{1/2}QA_+^{1/2}\leqslant A_+$ so that by taking spectral projections we get the result. Only the first term on the r.h.s. of (5.10) survives the $R\to 0$ limit. It tends to $W_{\hat{R}}\dfrac{\alpha p}{p^2}W_{\hat{R}}$. Therefore the spectral projection in Lemma (5.6) converges strongly. Since the vanishing term in (5.10) is negative $(\beta-1\leqslant 0)$ we can apply Lemma 1.23 [9, p. 438] and obtain norm convergence, completing the proof of Lemma (5.6).

The virture of Lemma (5.6) is that it tells us what the limiting points of the eigenvalues of $W_{R,\sigma}(H_0+1)^{-1}W_{R,\sigma}$ are (as $R\to 0$), namely the eigenvalues of $W_{\hat{R}}\dfrac{\alpha p}{p^2}W_{\hat{R}}$. The x-space kernel of this operator is

$$\left(\frac{1}{|x|}+\frac{1}{|x-\hat{R}|}\right)^{1/2}\frac{\alpha(x-y)}{|x-y|^3}\left(\frac{1}{|x|}+\frac{1}{|x-\hat{R}|}\right)^{1/2} \tag{5.11}$$

We suspect that

Conjecture. $\sigma\left(W_{\hat{R}}\frac{\alpha p}{p^2}W_{\hat{R}}\right)\cap((-\infty,-2)\cup(2,\infty))=\emptyset.$

A proof of this conjecture would rule out the occurrence of critical coupling constants. In fact, let $\lambda_1\geqslant\lambda_2\geqslant\cdots(\lambda_i>2)$ be the (positive) discrete eigenvalues of the above operator. Then the main theorem of this section is

Theorem (5.7). *Suppose $\mu\neq\lambda_i^{-1}$ $(i=1\cdots)$. Then $H(\mu,R)\to H(2\mu)$ in norm resolvent sense.*

Proof. Define $\delta=\operatorname{dist}\left[1,\sigma\left(\mu W_{\hat{R}}\frac{\alpha p}{p^2}W_{\hat{R}}\right)\right]>0$. Then $\delta\leqslant 1-2\mu$ by Lemma (5.5)(v). Choose σ so large that for all small enough R

$$\mu\,\|W_RH_0^{-1}W_R-W_{R,\sigma}H_0^{-1}W_{R,\sigma}\|\leqslant\delta/4 \tag{5.12}$$

Such a choice is possible, since the norm is bounded by const./$\sqrt{\sigma}$ independent of R. By Lemma (5.6) we may further assume that

$$\operatorname{dist}[1,\sigma(\mu W_{R,\sigma}(H_0+1)^{-1}W_{R,\sigma})]\geqslant 3\delta/4 \tag{5.13}$$

for sufficiently small R. Now we hop from $E=-1$ to $E=0$. The difference

$$W_{R,\sigma}((H_0+1)^{-1}-H_0^{-1})W_{R,\sigma}=W_{R,\sigma}\left(\frac{\alpha p}{p^2(p^2+1)}+\frac{\beta-1}{p^2}-\frac{\beta}{p^2+1}\right)W_{R,\sigma} \tag{5.14}$$

is compact. This follows from Lemma (5.4), which shows that (5.14) is the norm limit, as $E\downarrow-1$, of a compact operator. Moreover (5.14) tends in norm to a limit as $R\to 0$. To this end note that

$$|W_{R,\sigma}-W_{0,\sigma}|\leqslant\text{const.}\,|R|^{\delta}\left(\frac{1}{|x|^{1/2+\delta}}+\frac{1}{|x-R|^{1/2+\delta}}\right) \tag{5.15}$$

where $\delta\in(0,\frac{1}{2})$. Then use the $|p|$-boundedness of $\chi_0(x)\,|x|^{-(1/2+\delta)}$. Let K_R denote the operator in (5.13) and K_R^0 this operator at $E=0$. Let $D_R=K_R^0-K_R$. Then we know that: $[1-3\delta/4,1+3\delta/4]\in\rho(K_R)$ (5.13), $\sigma(K_0^0)=[-2\mu,2\mu]$ Lemma (5.5(iii)), D_R is compact. As $R\to 0$, $K_R^0\to K_0^0$ in norm, $D_R\to D_0$ in norm, $K_R\to K_0$ strongly. We wish to conclude that $1\in\rho(K_R^0)$ for sufficiently small R. In fact, we claim

$$\left(1-\frac{\delta}{2},1+\frac{\delta}{2}\right)\in\rho(K_R^0) \tag{5.16}$$

for all sufficiently small R. This is easily seen to be true if we realize that we are in a situation similar to the one in (4.13)–(4.19). Note that $\lambda\in(1-\delta/2,1+\delta/2)$ is eigenvalue of K_R^0 if and only if $(\lambda-K_R)^{-1}D_R$ has eigenvalue 1. This operator is norm continuous. Since 1 is not eigenvalue for $R=0$, (5.16) follows from a perturbation argument. Removing the cut-off σ using (5.12) yields

$$\left(1-\frac{\delta}{4},1+\frac{\delta}{4}\right)\in\rho(K_R^0)$$

for all sufficiently small R. Recalling (4.20) and proceeding as in the proof of Theorem (4.2) completes the proof.

Remark. Suppose $\mu = \lambda_i^{-1}$ for some i. Then $U_{|R|} W_R (H_0 - E)^{-1} W_R U^*_{|R|} \xrightarrow{R \to 0} W_{\hat{R}}(\alpha p/p^2) W_{\hat{R}}$ strongly for any $E \in \rho(H_0)$. For $E \in (-1, 1)$ this implies the existence of a sequence of eigenvalues τ_R of $W_R(H_0 - E)^{-1} W_R$ such that $\tau_R \to \lambda_i$ as $R \to 0$. Thus $\mu \cdot \tau_R \to 1$ and hence $\|(1 - K_R(E))^{-1}\| \to \infty$. Therefore our proof would break down.

5.4. $\mu > \frac{1}{2}$

The behavior of the eigenvalues when two centers with $\mu > \frac{1}{2}$ approach each other is spectacular. This is contained in the next theorem, which expresses the fact that an infinite number of eigenvalues passes through *any* point in the gap $(-1, 1)$ as $R \to 0$.

Theorem (5.8). *Suppose* $\mu \in (\frac{1}{2}, 1)$. *Let* $S_{E,r} = \{R \mid |R| < r,\ E \in \sigma(H(\mu, R))\}$. *Then, for any* $E \in (-1, 1)$ *and any* $r > 0$, $S_{E,r}$ *is an* infinite *set.*

Proof. Pick $E \in (-1, 1)$. Let $K_R(E) = \mu V_R^{1/2}(H_0 - E)^{-1} V_R^{1/2}$. Define $g(R) = \dim P_{(1,\infty)}(K_R(E))$. Since $\sigma_{\text{ess}}(K_R(E)) = [-\mu, \mu]$, $\sigma_{\text{ess}}(K_0(E)) = [-2\mu, 2\mu]$ where $2\mu > 1$ and $K_R(E) \to K_0(E)$ strongly, we conclude that $g(R) \to \infty$ as $R \to 0$ ([18, Thm. VIII 24]). Consider now a sequence $R_n = (z_n, 0, 0)$ $(z_n < r)$ such that $z_n \downarrow 0$ and $g(R_{n+1}) > g(R_n)$. Let $t_i(R)$ $(i = 1, 2, \ldots)$ denote, in descending order, the eigenvalues of $K_R(E)$ which are bigger than μ. On each interval $[z_n, z_{n+1}]$ consider the function $z \to t_s(R(z))$ where $R = (z, 0, 0)$ and $s = g(R_{n+1})$. $t_s(R(z))$ is continuous since, by a scale transformation, $K_R(E)$ is unitarily equivalent to

$$V_{\hat{R}}^{1/2} \frac{\alpha p + \beta\,|R| - E\,|R|}{p^2 + R^2(1 - E^2)} V_{\hat{R}}^{1/2}, \qquad \hat{R} = (1, 0, 0)$$

which is norm continuous in R for $R \neq 0$. But $t_s(R_n) < 1$ while $t_s(R_{n+1}) > 1$. Thus $t_s(R(z_n^*)) = 1$ at some point $z_n^* \in [z_n, z_{n+1}]$. Then $z_n^* \in S_{E,r}$. Doint this for all n proves the theorem.

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Appendix. The spectra of $\frac{1}{|x|}\frac{\alpha p}{p^2}$ **and** $\frac{1}{\sqrt{|x|}}\frac{\alpha p}{p^2}\frac{1}{\sqrt{|x|}}$.

a) $\frac{1}{|x|}\frac{\alpha p}{p^2}$: The operator admits a complete family of reducing subspaces, indexed by $\kappa = \pm 1, \pm 2 \ldots$

On these subspaces we have the representations

$$\alpha p: \begin{pmatrix} 0 & -\dfrac{d}{dx}+\dfrac{\kappa}{x} \\ \dfrac{d}{dx}+\dfrac{\kappa}{x} & 0 \end{pmatrix} \tag{A.1}$$

$$p^2: \begin{pmatrix} \dfrac{-d^2}{dx^2}+\dfrac{\kappa(\kappa+1)}{x^2} & 0 \\ 0 & \dfrac{-d^2}{dx^2}+\dfrac{\kappa(\kappa-1)}{x^2} \end{pmatrix} \equiv \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \tag{A.2}$$

on $[L^2(0,\infty)]^2$.

In the following we only consider $\kappa > 0$. The inverses of A and B have kernels

$$A^{-1}: \frac{1}{2\kappa+1}[\min(x, y)]^{\kappa+1}/[\max(x, y)]^{\kappa} \tag{A.3}$$

$$B^{-1}: \frac{1}{2\kappa-1}[\min(x, y)]^{\kappa}/[\max(x, y)]^{\kappa-1}$$

Hence

$$\frac{1}{|x|}\frac{\alpha p}{p^2}: \begin{pmatrix} 0 & x^{-\kappa-1}y\theta(x-y) \\ x^{\kappa-1}y^{-\kappa}\theta(y-x) & 0 \end{pmatrix} \tag{A.4}$$

where $\theta(x)=1$ resp. 0 if $x>1$ resp. $x<0$.

This operator commutes with dilations. By the unitary transformation

$U: [L^2(0,\infty)]^2 \to [L^2(-\infty,\infty)]^2$

$(Uf_1)(t) = e^{t/2}f_i(e^t) \qquad i=1,2$

(A.1) goes over into

$$\begin{pmatrix} 0 & e^{-(t-t')(\kappa+1/2)}\theta(t-t') \\ e^{-(t'-t)(\kappa-1/2)}\theta(t'-t) & 0 \end{pmatrix}$$

This operator commutes with translations. Performing a Fourier transform gives

$$\begin{pmatrix} 0 & \dfrac{1}{\kappa+\frac{1}{2}-ik} \\ \dfrac{1}{\kappa-\frac{1}{2}+ik} & 0 \end{pmatrix} \qquad k \in \mathbb{R} \tag{A.5}$$

So $\sigma\left(\dfrac{1}{|x|}\dfrac{\alpha p}{p^2}\right)$ is given by the values of the function

$$\xi_\kappa(k) = \left[\frac{(\kappa^2-\frac{1}{4}+k^2)-ik}{(\kappa^2-\frac{1}{4}+k^2)^2+k^2}\right]^{1/2}, \qquad k \in \mathbb{R} \tag{A.6}$$

Both branches of the square root have to be taken. The same formula holds for $\kappa<0$. $\xi_\kappa(k)$ is reflection symmetric with respect to the real and imaginary axis. Moreover

$$\xi_\kappa(0)=\pm\frac{1}{(\kappa^2-\frac{1}{4})} \tag{A.7}$$

and

$$\xi_\kappa^2(k)=re^{i\beta} \tag{A.8}$$

where

$$r=\frac{1}{(\kappa^2-\frac{1}{4}+k^2)^2+k^2} \tag{A.9}$$

$$\tan\beta=\left(\frac{rk^2}{1-rk^2}\right)^{1/2} \tag{A.10}$$

(A.9), (A.10) imply

$$\frac{\partial(\tan\beta)}{\partial\kappa}=\frac{\partial t(\tan\beta)}{\partial k}\frac{\partial k}{\partial\kappa}<0 \tag{A.11}$$

which shows that the curve $\xi_\kappa(k)$ encloses the curve $\xi_{\kappa'}(k)$ when $|\kappa'|>|\kappa|$.

b) $\dfrac{1}{\sqrt{|x|}}\dfrac{\alpha p}{p^2}\dfrac{1}{\sqrt{|x|}}$: The analog to (A.5) is

$$\begin{pmatrix} 0 & \dfrac{1}{\kappa-ik} \\ \dfrac{1}{\kappa+ik} & 0 \end{pmatrix} \tag{A.12}$$

The spectrum is the interval $[-1/\kappa, 1/\kappa]$.

Remark. It is tempting to conclude from (A.6) that the spectrum of $B=(1/|x|)(\alpha p/p^2)$ is contained in the circle of radius 4/3. However this is not allowed because we have a direct sum over *infinitely* many *non*self-adjoint operators. To be able to draw the desired conclusion it suffices to prove that $\|B_\kappa\|\to 0$ as $|\kappa|\to\infty$. Now $\|B_\kappa\|^2=\|B_\kappa^*B_\kappa\|=\|(|x|^{-1}p^{-2}|x|^{-1})_\kappa\|$. $(|x|^{-1}p^{-2}|x|^{-1})_\kappa$ is a diagonal (2×2) matrix operator. Its two entries are the restrictions to angular momentum $l=|\kappa|$ and $l=|\kappa|-1$ of the operator $|x|^{-1}p^{-2}|x|^{-1}$ on $L^2(\mathbb{R}^3)$. Using dilations one shows that on the subspace l this operator has as its spectrum the whole interval $[-4/(2l+1)^2, 4/(2l+1)^2]$, proving $\|B_\kappa\|\to 0$ as $|\kappa|\to\infty$.

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