Deficiency indices and singular boundary conditions in quantum mechanics

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We consider Schrödinger operators H in $L^2(\mathbb{R}^n)$, $n \in \mathbb{N}$, with countably infinitely many local singularities of the potential which are separated from each other by a positive distance. It is proved that due to locality each singularity yields a separate contribution to the deficiency index of H. In the special case where the singularities are pointlike and the potential exhibits certain symmetries near these points we give an explicit construction of self-adjoint boundary conditions.

I. INTRODUCTION

Our interest in the computation of deficiency indices and in the construction of self-adjoint boundary conditions for singular Schrödinger operators stems from several investigations of certain idealized model Hamiltonians, so-called point interactions.[1-10]

These analytically solvable models have a long history and play an important role in nuclear and solid state physics (cf., e.g., Ref. 9 and the literature therein). In this paper we particularly study the mathematical structure behind point interactions and some of their generalizations (interactions concentrated on submanifolds).

In Sec II we consider Schrödinger operators H in $L^2(\mathbb{R}^n)$, $n \in \mathbb{N}$ with countably infinitely many local singularities of the potential V which are uniformly separated from each other by a distance $\epsilon > 0$. Our main result (Theorem 2.5) concerning the deficiency index of H confirms the intuitive statement that due to locality each singularity should separately yield a contribution to the total deficiency index of H. Our proof is patterned after a result of Behncke[11] (c.f. also Ref. 12) where the corresponding problem is solved for strongly singular Dirac operators. Theorem 2.5 is general enough not only to include the case of point interactions in addition to V but also to allow additional interactions concentrated on submanifolds (like δ-shell interactions[8(b)]).

Section II represents the first step in the analysis, namely to reduce the computation of the deficiency indices of a Schrödinger operator H with several singularities to that of several Schrödinger operators H_j with a single singularity. The second step, the explicit construction of self-adjoint boundary conditions for H_j, is studied in Sec. III. In the special case where the singularity in H_j is pointlike and H_j exhibits certain symmetries around this point such that H_j reduces to a direct sum of ordinary Schrödinger operators in $L^2((0,\infty))$ (a case particularly important in applications) a general treatment of singular boundary conditions at the origin is presented. In particular, we study systems of the type

$$\frac{-d^2}{dr^2} + \frac{\lambda(\lambda-1)}{r^2} + \frac{\gamma}{r} + \frac{\alpha}{r^a} + W(r), \quad r > 0, \qquad (1.1)$$

with $W \in L^\infty((0,\infty))$ real valued, $\frac{1}{2} \le \lambda < \frac{3}{2}$, $\alpha, \gamma \in \mathbb{R}$, $0 < a < 2$.

Our methods rely heavily on the use of (ir)regular solutions associated with (1.1) and on corresponding Volterra integral equations. This yields a generalization of previous results of Rellich,[13] where the case $\alpha = 0$ in (1.1) has been considered.

II. DEFICIENCY INDICES OF SINGULAR SCHRÖDINGER OPERATORS

In this section we show that countably infinitely many local singularities of the potential which are uniformly separated from each other by a distance $\epsilon > 0$ do not interfere when considering the total deficiency index of the corresponding Schrödinger operator.

We introduce the following.

Hypothesis H: Let $J \subset \mathbb{Z} \setminus \{0\}$ be a finite or countably infinite index set, $J_0 = J \cup \{0\}$.

(i) $\Sigma_j \subset \mathbb{R}^n$, $n \in \mathbb{N}$ is a compact set of Lebesgue measure zero for all $j \in J$, $\Sigma_0 = \varnothing$.

(ii) $V_j \in L^2_{\rm loc}(\mathbb{R}^n \setminus \Sigma_j)$ is real valued, $j \in J_0$, and (a) supp (V_j) is compact for all $j \in J$, or (b) V_j are bounded from below on every compact subset of $\mathbb{R}^n \setminus \Sigma_j$ for all $j \in J_0$.

(iii) For some $\epsilon > 0$: $\operatorname{dist}(\{\operatorname{supp}(V_j) \cup \Sigma_j\}, \{\operatorname{supp}(V_{j'}) \cup \Sigma_{j'}\}) \ge \epsilon$ for all $j, j' \in J_0, j \ne j'$.

(iv) $W \in L^\infty(\mathbb{R}^n)$ is real-valued.

For notational convenience we will also use the abbreviations

$$A_j = \begin{cases} \operatorname{supp}(V_j) \cup \Sigma_j \text{ if condition H(ii)(a) holds,} \\ \Sigma_j \text{ if condition H(ii)(b) or conditions} \\ \quad \text{H(ii)(a) and H(ii)(b) hold}, \quad j \in J_0, \end{cases} \qquad (2.1)$$

$$A = \bigcup_{j \in J_0} A_j, \quad \Sigma = \bigcup_{j \in J_0} \Sigma_j, \quad V(x) = \sum_{j \in J_0} V_j(x),$$

and note that Σ is closed and of Lebesgue measure zero by hypotheses H(i) and H(iii).

As our first technical result we state the following.

Lemma 2.1: Assume conditions H(i) and H(iii). Then there exist $\phi_j, \tilde{\phi}_j \in C^\infty(\mathbb{R}^n)$, $j \in J_0$ such that we have the following.

(i) $\partial^\alpha \phi_j \in L^\infty(\mathbb{R}^n)$, $0 \leqslant |\alpha| \leqslant 2$, $\phi_j|_{A_j} = 1$, $j \in J_0$.

(ii) $\operatorname{supp}(\phi_j) \cap \operatorname{supp}(\phi_{j'}) = \varnothing$, $j, j' \in J_0$, $j \ne j'$.

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(iii) For some $0<\delta<\epsilon/2$: $\text{dist}(\text{supp}(1-\phi_j),A_j)\geqslant\delta$, $j\in J_0$.

(iv) $\partial^\alpha\tilde{\phi}_j\in L^\infty(\mathbb{R}^n)$, $0\leqslant|\alpha|\leqslant 2$, $\tilde{\phi}_j|_{\text{supp}(\phi_j)}=1$, $j\in J_0$.

(v) $\text{supp}(\tilde{\phi}_j)\cap\text{supp}(\tilde{\phi}_{j'})=\varnothing$, $j,j'\in J_0$, $j\neq j'$.

(vi) $\phi_0(x)=1$ for $x\in\{y\in\mathbb{R}^n\mid |y|\geqslant R\}$ for some $R>0$ if condition H(ii)(a) holds, and $\phi_j\in C_0^\infty(\mathbb{R}^n)$ and $\text{dist}(\text{supp}(\phi_j),\text{supp}(V_{j'}))\geqslant\delta$ for all $j,j'\in J_0, j\neq j'$ if condition H(ii)(b) holds.

Proof: Fix $l\in J_0$ and define

$$U_{l,\eta}=\bigcup_{a\in A_l}S(a;\eta),\quad \eta>0. \tag{2.2}$$

[$S(x_0;R)$ is the open ball of radius R centered at x_0.] Then $U_{l,\epsilon/32}$ is an open neighborhood of A_l. If we introduce

$$E_{l,\epsilon/32}=\overline{U_{l,\epsilon/32}},\quad F_{l,\epsilon/16}=\mathbb{R}^n\setminus U_{l,\epsilon/16}, \tag{2.3}$$

then $E_{l,\epsilon/32}$ and $F_{l,\epsilon/16}$ are closed and disjoint and we can apply Corollary 1.4.11 of Ref. 14 to get the existence of $\phi_l\in C^\infty(\mathbb{R}^n)$ such that

$$\phi_l|_{E_{l,\epsilon/32}}=1,\quad \phi_l|_{F_{l,\epsilon/16}}=0,$$
$$\partial^\alpha\phi_l\in L^\infty(\mathbb{R}^n),\quad 0\leqslant|\alpha|\leqslant 2. \tag{2.4}$$

The collection of all such ϕ_l, $l\in J_0$ obviously fulfills assertions (i)–(vi) (with $\delta\geqslant\epsilon/32$). For the construction of $\tilde{\phi}_j, j\in J_0$ one simply replaces ϵ by 3ϵ.

For the rest of this section ϕ_j (resp. $\tilde{\phi}_j$) always denote the $C^\infty(\mathbb{R}^n)$ functions of Lemma 2.1. Next we introduce the minimal Schrödinger operators

$$\dot{H}_j=-\Delta+V_j\ \text{ on }\ \mathscr{D}(\dot{H}_j)=C_0^\infty(\mathbb{R}^n\setminus\Sigma_j),\quad j\in J_0, \tag{2.5}$$

$$\dot{H}=-\Delta+V+W\ \text{ on }\ \mathscr{D}(\dot{H})=C_0^\infty(\mathbb{R}^n\setminus\Sigma), \tag{2.6}$$

and denote their closures by

$$H_j=\overline{\dot{H}_j},\quad H=\overline{\dot{H}}. \tag{2.7}$$

Due to hypotheses H(i), H(ii), and H(iv) the corresponding adjoint operators read

$$\begin{aligned}H_j^*g=&-\Delta g+V_jg\ \text{ in }\ C_0^\infty(\mathbb{R}^n\setminus\Sigma_j)',\\ &\text{for } g\in\mathscr{D}(H_j^*)=\{f\in L^2(\mathbb{R}^n)\mid-\Delta f\\ &\qquad+V_jf\in L^2(\mathbb{R}^n)\},\quad j\in J_0,\end{aligned} \tag{2.8}$$

$$\begin{aligned}H^*g=&-\Delta g+(V+W)g\ \text{ in }\ C_0^\infty(\mathbb{R}^n\setminus\Sigma)',\\ &\text{for } g\in\mathscr{D}(H^*)=\{f\in L^2(\mathbb{R}^n)\mid-\Delta f\\ &\qquad+(V+W)f\in L^2(\mathbb{R}^n)\}.\end{aligned} \tag{2.9}$$

We start our analysis with the following.

Lemma 2.2: Assume hypotheses H(i)–H(iv). Then, for all $j\in J_0$,

$$\text{(i) } g\in\mathscr{D}(H_j^*)\ \text{ implies }\ \phi_j\,g\in\mathscr{D}(H_j^*)\cap\mathscr{D}(H^*), \tag{2.10}$$

$$\text{(ii) } g\in\mathscr{D}(H^*)\ \text{ implies }\ \phi_j\,g\in\mathscr{D}(H^*)\cap\mathscr{D}(H_j^*), \tag{2.11}$$

and $H^*(\phi_j\,g)=H_j^*(\phi_j\,g)+W(\phi_j\,g)$ in both cases.

Proof: (a) Suppose condition H(ii)(a) to be valid. Then we first prove

$$\mathscr{D}(H_j^*)\subset H^{2,2}_{\text{loc}}(\mathbb{R}^n\setminus\{\text{supp}(V_j)\cup\Sigma_j\}),\quad j\in J_0, \tag{2.12}$$

$$\mathscr{D}(H^*)\subset H^{2,2}_{\text{loc}}(\mathbb{R}^n\setminus\{\text{supp}(V)\cup\Sigma\}). \tag{2.13}$$

Let $g\in\mathscr{D}(H_j^*)$, $\psi_j\in C_0^\infty(\mathbb{R}^n\setminus A_j)$. Then $H_j^*g=-\Delta g+V_jg\in L^2(\mathbb{R}^n)$ implies $\psi_j(H_j^*g)=-\psi_j(\Delta g)\in L^2(\mathbb{R}^n)$ and by the arbitrariness of ψ_j we infer $\Delta g\in L^2_{\text{loc}}(\mathbb{R}^n\setminus A_j)$. By Theorem 1 of Ref. 15 we get $\nabla g\in L^2_{\text{loc}}(\mathbb{R}^n\setminus A_j)$ and hence relation (2.12) results. Similarly $g\in\mathscr{D}(H^*)$, $\psi\in C_0^\infty(\mathbb{R}^n\setminus A)$ implies $\psi(H^*g)=-\psi(\Delta g)+\psi Wg\in L^2(\mathbb{R}^n)$ and hence relation (2.13) follows. If condition H(ii)(b) holds then again $\nabla g\in L^2_{\text{loc}}(\mathbb{R}^n\setminus A_j)$ for $g\in\mathscr{D}(H_j^*)$ and $\nabla g\in L^2_{\text{loc}}(\mathbb{R}^n\setminus A)$ for $g\in\mathscr{D}(H^*)$ by Theorem 1 of Ref. 15.

(b) Let $g\in\mathscr{D}(H_j^*)$. Then

$$\begin{aligned}(-\Delta+V_j+W)(\phi_j\,g)&=(-\Delta+V+W)(\phi_j\,g)\\&=\phi_j(-\Delta+V_j+W)g-2(\nabla\phi_j)(\nabla g)\\&\quad-(\Delta\phi_j)g\in L^2(\mathbb{R}^n),\end{aligned}$$

since ϕ_j, $\Delta\phi_j\in L^\infty(\mathbb{R}^n)$, $\nabla\phi_j\in C_0^\infty(\mathbb{R}^n\setminus A)$, and $\nabla g\in L^2_{\text{loc}}(\mathbb{R}^n\setminus A_j)$ by (a).

(c) Let $g\in\mathscr{D}(H^*)$. Then

$$\begin{aligned}(-\Delta+V+W)(\phi_j\,g)&=(-\Delta+V_j+W)(\phi_j\,g)\\&=\phi_j(-\Delta+V+W)g-2(\nabla\phi_j)(\nabla g)\\&\quad-(\Delta\phi_j)g\in L^2(\mathbb{R}^n),\end{aligned}$$

since ϕ_j, $\Delta\phi_j\in L^\infty(\mathbb{R}^n)$, $\nabla\phi_j\in C_0^\infty(\mathbb{R}^n\setminus A)$, and $\nabla g\in L^2_{\text{loc}}(\mathbb{R}^n\setminus A)$ by (a). ∎

Lemma 2.3: Assume conditions H(i)–H(iv). Then, for all $j\in J_0$,

$$g\in\mathscr{D}(H)\ \text{ implies }\ \phi_jg\in\mathscr{D}(H)\cap\mathscr{D}(H_j) \tag{2.14}$$

and $H(\phi_j\,g)=H_j(\phi_j\,g)+W(\phi_j\,g)$.

Proof: Let $g\in\mathscr{D}(H)$. Then there exists a sequence

$$\{g_m\}_{m\in\mathbb{N}}\subset C_0^\infty(\mathbb{R}^n\setminus\Sigma),$$

$$\text{such that }\ g_m\xrightarrow[m\to\infty]{s}g,\quad \dot{H}g_m\xrightarrow[m\to\infty]{s}Hg.$$

Consequently, $\phi_j\,g_m\in C_0^\infty(\mathbb{R}^n\setminus\Sigma)$, $\phi_j\,g_m\xrightarrow[m\to\infty]{s}\phi_j\,g$, and

$$\begin{aligned}\dot{H}(\phi_j\,g_m)&=(-\Delta+V_j+W)(\phi_j\,g_m)\\&=\phi_j(-\Delta+V+W)g_m-2(\nabla\phi_j)(\nabla g_m)\\&\quad-(\Delta\phi_j)g_m.\end{aligned} \tag{2.15}$$

Since

$$\phi_j(-\Delta+V+W)g_m\xrightarrow[m\to\infty]{s}\phi_jHg,\quad(\Delta\phi_j)g_m\xrightarrow[m\to\infty]{s}(\Delta\phi_j)g, \tag{2.16}$$

it remains to consider the second term on the right-hand side of (2.15).

Let $\psi\in C_0^\infty(\mathbb{R}^n\setminus A)$ be real valued. Then $g\in H^{2,2}_{\text{loc}}(\mathbb{R}^n\setminus A)$ implies

$$\begin{aligned}\int_{\mathbb{R}^n}d^nx\,\psi^2|\nabla(g_m-g)|^2&=-2\int_{\mathbb{R}^n}d^nx\,\overline{(g_m-g)}(\nabla\psi)\psi\nabla(g_m-g)\\&\quad-\int_{\mathbb{R}^n}d^nx\,\overline{(g_m-g)}\psi^2\Delta(g_m-g),\end{aligned} \tag{2.17}$$

and thus

$$\|\psi|\nabla(g_m-g)|\,\|_2\leqslant 2\|\,|\nabla\psi|\,\|_\infty\|g_m-g\|_2\|\psi|\nabla(g_m-g)|\,\|_2 + \|g_m-g\|\,\|\psi^2\Delta(g_m-g)\|_2. \quad (2.18)$$

Inequality (2.18) proves $\|\psi|\nabla(g_m-g)|\,\|_2 \underset{m\to\infty}{\longrightarrow} 0$. By taking $\psi_p^2=|\partial_p\phi_j|^2$, $p=1,...,n$ we infer $\|(\partial_p\phi_j)|\nabla(g_m-g)|\,\|_2 \underset{m\to\infty}{\longrightarrow} 0$ and hence also

$$\|(\nabla\phi_j)\nabla(g_m-g)\|_2 \underset{m\to\infty}{\longrightarrow} 0,\quad j\in J_0. \quad (2.19)$$

Consequently,

$$\dot H(\phi_j g_m)=\dot H_j(\phi_j g_m)+W(\phi_j g_m) \overset{s}{\underset{m\to\infty}{\longrightarrow}} \phi_j Hg-2(\nabla\phi_j)\nabla g-(\Delta\phi_j)g. \quad (2.20)$$

Since H and H_j are closed we get from Eqs. (2.15), (2.16), and (2.20) $\phi_j g\in\mathscr{D}(H)\cap\mathscr{D}(H_j)$,

$$H(\phi_j g)=H_j(\phi_j g)+W(\phi_j g) = \phi_j Hg-2(\nabla\phi_j)(\nabla g)-(\Delta\phi_j)g. \qquad ■$$

Lemma 2.4: Assume hypotheses H(i)–H(iv). Then, for all $j\in J_0$,

(i) $g\in\mathscr{D}(H_j^*)$ implies $(1-\phi_j)g\in\mathscr{D}(H_j)$, (2.21)

(ii) $g\in\mathscr{D}(H^*)$ implies $\left(1-\sum_{j\in J_0}\phi_j\right)g\in\mathscr{D}(H)$. (2.22)

Proof: (a) Let $g\in\mathscr{D}(H_j^*)$. Then $(1-\phi_j)g\in\mathscr{D}(H_j^*)$ by Lemma 2.2 (i). Denote $\psi_j=1-\phi_j$: then $H_j^*(\psi_j g) = -\Delta(\psi_j g)$ in $C_0^\infty(\mathbb{R}^n\setminus\Sigma_j)'$ implies $-\Delta(\psi_j g)\in L^2(\mathbb{R}^n)$ and hence $\psi_j g\in H^{2,2}(\mathbb{R}^n)$. Let

$$0\leqslant\chi\in C_0^\infty(\mathbb{R}^n),\quad |\partial^\alpha\chi|\leqslant M<\infty,$$
$$0\leqslant|\alpha|\leqslant 2,\quad \chi(x)=\begin{cases}1, & |x|\leqslant 1,\\ 0, & |x|\geqslant 2,\end{cases} \quad (2.23)$$
$$\chi_R(x)=\chi(xR^{-1}),\quad R>0,$$

and

$$0\leqslant j\in C_0^\infty(\mathbb{R}^n),\quad j(x)=0,\quad |x|\geqslant 1,\quad \int_{\mathbb{R}^n}d^nx\,j(x)=1, \quad (2.24)$$

$$j_\epsilon(x)=\epsilon^{-n}j(x/\epsilon),\quad \epsilon>0.$$

Then

$$\psi_j g\chi_R * j_{R^{-1}}\in C_0^\infty(\mathbb{R}^n\setminus A_j),\quad \text{for } R>0 \text{ large enough} \quad (2.25)$$

and

$$\psi_j g\chi_R * j_{R^{-1}} \overset{H^{2,2}(\mathbb{R}^n\setminus A_j)}{\underset{R\to\infty}{\longrightarrow}} \psi_j g. \quad (2.26)$$

Thus, $\psi_j g\in H_0^{2,2}(\mathbb{R}^n\setminus A_j)$. Consequently there exists a sequence

$\{f_m\}_{m\in\mathbb{N}}\subset C_0^\infty(\mathbb{R}^n\setminus A_j)$, such that

$f_m \underset{m\to\infty}{\longrightarrow} \psi_j g$ in $H^{2,2}(\mathbb{R}^n\setminus A_j)$ norm. This proves

$$\dot H_j f_m=-\Delta f_m \overset{s}{\underset{m\to\infty}{\longrightarrow}} -\Delta(\psi_j g),$$

and hence

$$\psi_j g\in\mathscr{D}(H_j)\quad\text{and}\quad H_j(\psi_j g)=-\Delta(\psi_j g), \quad (2.27)$$

since H_j is closed.

(b) Let $g\in\mathscr{D}(H^*)$, $\Psi=1-\Sigma_{j\in J_0}\phi_j$. Then $\Psi g\in H_0^{2,2}(\mathbb{R}^n\setminus A)$ as above and (2.22) follows. ■

Given Lemmas 2.2–2.4, we are able to state the main result of this section.

Theorem 2.5: Assume conditions H(i)–H(iv). Then

$$\operatorname{def}(H)=\sum_{j\in J_0}\operatorname{def}(H_j). \quad (2.28)$$

Proof: We first assume that $\operatorname{def}(H_j)<\infty$ for all $j\in J_0$.

(a) Let $\{\Phi_{jl}\in\mathscr{D}(H_j^*),\ 1\leqslant l\leqslant 2\operatorname{def}(H_j)\}$ be linearly independent modulo $\mathscr{D}(H_j)$, $j\in J_0$. (We note that the deficiency indices of H_j coincide since V_j is real valued.) By Lemma 2.2 (i) we get

$$\phi_j\Phi_{jl}\in\mathscr{D}(H_j^*)\cap\mathscr{D}(H^*),\quad 1\leqslant l\leqslant 2\operatorname{def}(H_j), j\in J_0. \quad (2.29)$$

Suppose there exist $\beta_{jl}\in\mathbb{C}$ such that

$$\sum_{j\in J_0}\sum_{l=1}^{2\operatorname{def}(H_j)}\beta_{jl}\,\phi_j\,\Phi_{jl}\in\mathscr{D}(H). \quad (2.30)$$

Then, by the locality of H,

$$\phi_j\sum_{l=1}^{2\operatorname{def}(H_j)}\beta_{jl}\,\Phi_{jl}\in\mathscr{D}(H),\quad j\in J_0, \quad (2.31)$$

since $\operatorname{supp}(\phi_j)\cap\operatorname{supp}(\phi_{j'})=\varnothing$ for $j,j'\in J_0, j\neq j'$. Now choose $\tilde\phi_j$ as in Lemma 2.1. Then Lemma 2.3 implies

$$\tilde\phi_j\left(\phi_j\sum_{l=1}^{2\operatorname{def}(H_j)}\beta_{jl}\,\Phi_{jl}\right) =\phi_j\sum_{l=1}^{2\operatorname{def}(H_j)}\beta_{jl}\,\Phi_{jl}\in\mathscr{D}(H_j),\quad j\in J_0. \quad (2.32)$$

On the other hand, from Lemma 2.4(i) we infer

$$(1-\phi_j)\sum_{l=1}^{2\operatorname{def}(H_j)}\beta_{jl}\,\Phi_{jl}\in\mathscr{D}(H_j),\quad j\in J_0, \quad (2.33)$$

and hence

$$\sum_{l=1}^{2\operatorname{def}(H_j)}\beta_{jl}\,\Phi_{jl}\in\mathscr{D}(H_j),\quad j\in J_0, \quad (2.34)$$

implying

$$\beta_{jl}=0,\quad 1\leqslant l\leqslant 2\operatorname{def}(H_j),\quad j\in J_0. \quad (2.35)$$

Thus, because of (2.31), $\{\phi_j\,\Phi_{jl},\ 1\leqslant l\leqslant 2\operatorname{def}(H_j), j\in J_0\}$ are linearly independent modulo $\mathscr{D}(H)$. Consequently,

$$2\operatorname{def}(H)=\dim\mathscr{D}(H^*)/\mathscr{D}(H)\geqslant 2\sum_{j\in J_0}\operatorname{def}(H_j). \quad (2.36)$$

(b) Conversely, let $\{\Psi_p\in\mathscr{D}(H^*),\ 1\leqslant p\leqslant 2\operatorname{def}(H)\}$ be linearly independent modulo $\mathscr{D}(H)$. By Lemma 2.4(ii) we get

$$\left(1-\sum_{j\in J_0}\phi_j\right)\Psi_p\in\mathscr{D}(H), \quad (2.37)$$

i.e.,

$$\Psi_p=\left(\sum_{j\in J_0}\phi_j\right)\Psi_p\quad\text{modulo } \mathscr{D}(H). \quad (2.38)$$

By Lemma 2.2(ii)

$$\phi_j \Psi_p \in \mathscr{D}(H^*) \cap \mathscr{D}(H_j^*), \quad j \in J_0, \tag{2.39}$$

and thus $\phi_j \Psi_p$ can be written

$$\phi_j \Psi_p = \Phi_{j0} + \sum_{l=1}^{2\,\mathrm{def}(H_j)} C_{pjl} \Phi_{jl}, \quad \Phi_{j0} \in \mathscr{D}(H_j),$$
$$C_{pjl} \in \mathbb{C}, \quad 1 \leqslant p \leqslant 2\,\mathrm{def}(H), \quad j \in J_0 \tag{2.40}$$

[i.e., $\phi_j \Psi_p = \Sigma_{l=1}^{2\,\mathrm{def}(H_j)} C_{pjl} \Phi_{jl}$ modulo $\mathscr{D}(H_j)$]. Since $1 \leqslant p \leqslant 2\,\mathrm{def}(H)$, we get from Eq. (2.38)

$$2\,\mathrm{def}(H) \leqslant 2 \sum_{j \in J_0} \mathrm{def}(H_j). \tag{2.41}$$

If $\mathrm{def}(H_j) = \infty$ for some $j \in J_0$ then it suffices to follow part (a) in order to conclude $\mathrm{def}(H) = \infty$. ∎

For the rest of this section we discuss hypotheses H(i)–H(iv) and sketch possible generalizations. We start with two examples which clearly demonstrate the range of applicability of Theorem 2.5.

Example 2.6: Let

$$V(x) + W(x) = \sum_{j=1}^{N} C_j^{(1)} |x - y_j|^{-\alpha_j} + \sum_{j=1}^{N} C_j^{(2)} |x - z_j|^{-\beta_j} \times (x - z_j) \cdot e_j + \sum_{j=1}^{N} C_j^{(3)} \| x - x_j| - R_j|^{-\gamma_j} + \sum_{j=1}^{N} C_j^{(4)} x^j, \tag{2.42}$$

where

$$C_j^{(l)} \in \mathbb{R}, \quad l = 1,...,4, \quad e_j \in \mathbb{R}^n, \quad |e_j| = 1,$$
$$x_j, y_j, z_j \in \mathbb{R}^n, \quad R_j > 0,$$
$$\{x \in \mathbb{R}^n |\ |x - x_j| \leqslant R_j\} \cap \{x \in \mathbb{R}^n |\ |x - x_{j'}| \leqslant R_{j'}\} = \varnothing, \quad j \neq j', \tag{2.43}$$
$$\{y_j, z_j, j = 1,...,N\} \cap \bigcup_{j'=1}^{N} \{x \in \mathbb{R}^n |\ |x - x_{j'}| = R_{j'}\} = \varnothing,$$
$$\alpha_j \geqslant 0, \quad \beta_j \geqslant 0, \quad \gamma_j \geqslant 0, \quad j, j' = 1,...,N, \quad N \in \mathbb{N}.$$

Thus one may choose

$$\Sigma = \bigcup_{j=1}^{N} (\{y_j\} \cup \{z_j\} \cup \{x \in \mathbb{R}^n |\ |x - x_j| = R_j\}). \tag{2.44}$$

Example 2.7: Let

$$V(x) + W(x) = \prod_{m=1}^{n} |\sin(\mu_m x_{(m)})|^{-\nu_m}, \tag{2.45}$$

where

$$x = (x_{(1)},...,x_{(n)}) \in \mathbb{R}^n, \quad \mu_m > 0, \quad \nu_m \geqslant 0, \quad m = 1,...,n, \tag{2.46}$$

and hence we choose

$$\Sigma = \left\{ \left(\frac{\pi p_1}{\mu_1},...,\frac{\pi p_n}{\mu_n} \right) \in \mathbb{R}^n | p_m \in \mathbb{Z}, m = 1,...,n \right\}. \tag{2.47}$$

Remark 2.8: The strategy in the proof of Theorem 2.5 is taken from that of Theorem 1(1) in Behncke[11] (cf. also Ref. 12), where the case of strongly singular Dirac operators (including, e.g., the anomalous magnetic moment term) is treated. In particular, Behncke discussed the case where the Σ_j are disjoint finite sets and also derived the invariance of essential spectra. For related results in the context of distinguished self-adjoint extensions for the Dirac operator with a potential dominated by multicenter Coulomb potentials we refer to Refs. 16.

The main ingredients for Theorem 2.5 are obviously relations (2.10), (2.11), (2.14), (2.21), and (2.22). [We also note that the existence of $\phi_j, \tilde{\phi}_j$ in Lemma 2.1 is clearly independent of the fact whether $A_j, j \in J$ are compact or not; only the fact that $\mathrm{dist}(A_j, A_{j'}) \geqslant \epsilon, j \neq j'$ has been used.[14]] In particular, the main technical difference between the Schrödinger case presented above and the Dirac case in Ref. 11 now concerns the necessity to control ∇g for $g \in \mathscr{D}(H_j^*)$ or $g \in \mathscr{D}(H^*)$ [i.e., to prove $\nabla g \in L^2_{\mathrm{loc}}(\mathbb{R}^n \setminus A_j)$ or $\nabla g \in L^2_{\mathrm{loc}}(\mathbb{R}^n \setminus A)$]. For example, if $V_j \in Q_{\alpha_j,\mathrm{loc}}(\mathbb{R}^n \setminus \{x_j\})$, $0 < \alpha_j \leqslant 1$ then $\mathscr{D}(H_j^*) \subset H^{2,2}_{\mathrm{loc}}(\mathbb{R}^n \setminus \{x_j\}) \cap L^2(\mathbb{R}^n)$ (Ref. 17) is obviously sufficient to prove Lemma 2.2–Theorem 2.5 (with $A_j = \Sigma_j = \{x_j\}$).

For related results on local properties of elements in $\mathscr{D}(H_j^*)$ we also refer to Pearson,[18] Combescure and Ginibre,[19] and Amrein.[20] Another particular important case where $\mathrm{def}(H_j) = \mathrm{def}(H) = 0$ appeared in Simader,[21] Brezis,[22] and Cycon.[23] Similarly, Morgan[24] used the idea of local partitions to prove stability of operator bounds and form bounds in the context of Schrödinger operators whose potentials have separated singularities. Finally, Svendsen[25] discussed the case where $A: C_0^\infty(\Omega, \mathbb{C}^s) \to L^2(\Omega, \mathbb{C}^s)$ is a linear symmetric differential operator with C^∞ coefficients, $\Omega \subset \mathbb{R}^n$ open, $n, s \in \mathbb{N}$. If M is a C^∞ manifold of Ω which is closed in Ω and has codimension greater than zero he studied the relation between the deficiency indices of A and $A|_{C_0^\infty(\Omega \setminus M, \mathbb{C}^s)}$.

We also mention the possibility of replacing $\mathbb{R}^n$ by $\Omega \subset \mathbb{R}^n$ open in the above treatment. The corresponding minimal operators are then given by $H_j = -\Delta + V_j$ on $C_0^\infty(\Omega \setminus \Sigma_j)$ and results on $\mathscr{D}(H_j^*)$ in this case may be found in Jörgens[26] and Kalf[15] and the references therein.

Theorem 2.5 relates the computation of $\mathrm{def}(H)$ to that of $\mathrm{def}(H_j), j \in J_0$. For the determination of deficiency indices of singular Schrödinger operators we refer to Piepenbrink and Rejto[27] and Behncke and Focke.[28] In the special case where $V_j(x) = V_j(|x - x_j|)$ is spherically symmetric [or H_j can be decomposed into a direct sum of ordinary differential operators like in the case of

$$V_j(x) = c_j |x - x_j|^{-3} (x - x_j) \cdot e_j,$$
$$x_j, e_j \in \mathbb{R}^n, \quad |e_j| = 1, \quad c_j \in \mathbb{R};$$

cf. Ref. 29], numerous methods to calculate the deficiency indices of the underlying ordinary differential operators are known.[30–32] In the special case

$$\Sigma = \{x_1,...,x_N\}, \quad x_j \in \mathbb{R}^n, \quad j = 1,...,N, \quad N \in \mathbb{N},$$

the corresponding deficiency subspaces have been obtained by Zorbas[33] with the help of suitable Green's functions.

III. SINGULAR BOUNDARY CONDITIONS FOR ORDINARY DIFFERENTIAL OPERATORS

In Sec. II we indicated how to reduce the computation of $\mathrm{def}(H)$ to that of $\mathrm{def}(H_j)$. In the special case where H_j can be decomposed into a direct sum of ordinary differential operators on $(0, \infty)$ [e.g.,

$$V_j(x) = v_j(|x - x_j|)$$

or

$$V_j(x) = c_j|x - x_j|^{-3}(x - x_j)\cdot e_j,$$
$$x_j, e_j \in \mathbb{R}^n, \quad |e_j| = 1, \quad c_j \in \mathbb{R}, \quad n \in N],$$

we now discuss possible self-adjoint boundary conditions at the origin. More precisely, we consider in $L^2((0,\infty))$ the minimal operator

$$\dot{h} = -\frac{d^2}{dr^2} + \frac{\lambda(\lambda-1)}{r^2} + \frac{\gamma}{r} + \frac{\alpha}{r^a} + W$$
$$\text{on } \mathscr{D}(\dot{h}) = C_0^\infty((0,\infty)),$$
$$W \in L^\infty((0,\infty)) \text{ real valued}, \ \alpha,\gamma \in \mathbb{R},$$
$$0 < a < 2, \quad \tfrac{1}{2} \leqslant \lambda < \tfrac{3}{2}. \tag{3.1}$$

As has been discussed in Refs. 2–10 and 34, self-adjoint extensions of $\dot{h}$ different from its Friedrichs extension correspond to a $\lambda(\lambda-1)r^{-2} + \gamma r^{-1} + \alpha r^{-a} + W +$ "point interaction." It is the purpose of this section to construct all self-adjoint extensions of $\dot{h}$

Due to our conditions on λ, the closure of $\dot{h}$, denoted by h, is bounded from below and has def$(h) = 1$. In order to determine explicitly the one-parameter family of self-adjoint extensions of h we shall study solutions of the equation

$$-\psi''(r) + [\lambda(\lambda-1)r^{-2} + V(r)]\psi(r) = 0, \quad r > 0, \tag{3.2}$$

where

$$V(r) = \gamma r^{-1} + \alpha r^{-a} + W(r). \tag{3.3}$$

Let $F_\lambda(r)$ be the regular solution of Eq. (3.2), i.e.,

$$F_\lambda(r) = F_\lambda^{(0)}(r) - \int_0^r dr'\, g_\lambda^{(0)}(r,r')V(r')F_\lambda(r'), \tag{3.4}$$

where

$$g_\lambda^{(0)}(r,r') = G_\lambda^{(0)}(r)F_\lambda^{(0)}(r') - G_\lambda^{(0)}(r')F_\lambda^{(0)}(r), \tag{3.5}$$
$$F_\lambda^{(0)}(r) = r^\lambda,$$
$$G_\lambda^{(0)}(r) = \begin{cases} -r^{1/2}\ln r, & \lambda = \frac{1}{2}, \\ (2\lambda-1)^{-1}r^{1-\lambda}, & \frac{1}{2} < \lambda < \frac{3}{2}. \end{cases} \tag{3.6}$$

We also note that $[G_\lambda^{(0)}, F_\lambda^{(0)}]_r = 1$, where $[g,f]_r = (\bar{g}, f' - \bar{g}'f)(r)$ denotes the Wronskian of g and f. Since $\int_0^R dr\, r|V(r)| < \infty$ for any $0 < R < \infty$ (needed in the case $\frac{1}{2} < \lambda < \frac{3}{2}$) as well as $\int_0^{r_0} dr\, r|\ln r|\,|V(r)| < \infty$ for all $0 < r_0 < 1$ (needed for $\lambda = \frac{1}{2}$), we may iterate Eq. (3.4) to get[35,36]

$$|F_\lambda(r)| \leqslant r^\lambda \begin{cases} \exp\left[\int_0^r dr'\, r'|V(r')|\right], & \frac{1}{2} < \lambda < \frac{3}{2}, \\ \exp\left[\int_0^r dr'\, r'|\ln r'|\,|V(r')|\right], & \lambda = \frac{1}{2}, \quad r \leqslant r_0, \end{cases}$$
$$\leqslant c r^\lambda. \tag{3.7}$$

Similarly, if

$$F_\lambda(r) = \sum_{m=0}^\infty F_\lambda^{(m)}(r) \tag{3.8}$$

denotes the absolute convergent series obtained by iterating Eq. (3.4), then

$$\left|F_\lambda(r) - \sum_{m=0}^N F_\lambda^{(m)}(r)\right| = \left|\int_0^r dr_1\, g_\lambda^{(0)}(r,r_1)V(r_1)\int_0^{r_1} dr_2\, g_\lambda^{(0)}(r_1,r_2)V(r_2)\cdots\int_0^{r_N} dr_{N+1}\, g_\lambda^{(0)}(r_N,r_{N+1})V(r_{N+1})F_\lambda(r_{N+1})\right|$$
$$\leqslant c[(N+1)!]^{-1}r^\lambda \begin{cases} \left[\int_0^r dr'\, r'|\ln r'|\,|V(r')|\right]^{N+1}, & \lambda = \frac{1}{2}, \quad r \leqslant r_0, \\ \left(\frac{2}{2\lambda-1}\right)^{N+1}\left[\int_0^r dr'\, r'|V(r')|\right]^{N+1}, & \frac{1}{2} < \lambda < \frac{3}{2}. \end{cases} \tag{3.9}$$

Here the estimate

$$|g_\lambda^{(0)}(r,r')| \leqslant \begin{cases} (rr')^{1/2}|\ln r'|, & \lambda = \frac{1}{2}, \quad r' \leqslant r \leqslant r_0 < 1, \\ [2/(2\lambda-1)]r^\lambda r'^{1-\lambda}, & \frac{1}{2} < \lambda < \frac{3}{2}, \end{cases} \tag{3.10}$$

has been used. Moreover,

$$\left|\int_0^r dr'\, g_\lambda^{(0)}(r,r')V(r')F_\lambda(r')\right|$$
$$\leqslant c r^\lambda \begin{cases} \int_0^r dr'\, r'|\ln r'|\,|V(r')|, & \lambda = \frac{1}{2}, \quad r \leqslant r_0, \\ \int_0^r dr'\, r'|V(r')||, & \frac{1}{2} < \lambda < \frac{3}{2}, \end{cases} \tag{3.11}$$

using (3.4) and (3.6), shows that

$$F_\lambda(r) = F_\lambda^{(0)}(r)[1 + \widehat{F}_\lambda(r)], \tag{3.12}$$

where

$$|\widehat{F}_\lambda(r)| \leqslant \begin{cases} c\int_0^r dr'\, r'|\ln r'|\,|V(r')|, & \lambda = \frac{1}{2}, \quad r \leqslant r_0, \\ c\int_0^r dr'\, r'|V(r')|, & \frac{1}{2} < \lambda < \frac{3}{2}, \end{cases} \tag{3.13}$$

and thus

$$\widehat{F}_\lambda(r) \underset{r\to 0_+}{=} o(1), \quad \tfrac{1}{2} \leqslant \lambda < \tfrac{3}{2}. \tag{3.14}$$

Consequently, we infer

$$|F_\lambda(r)| \leqslant c_1(r_0)|F_\lambda^{(0)}(r)| = c_1(r_0)r^\lambda,$$
$$|F_\lambda(r)| \geqslant c_2(r_0)|F_\lambda^{(0)}(r)| = c_2(r_0)r^\lambda,$$
$$\tfrac{1}{2} \leqslant \lambda < \tfrac{3}{2}, \quad r \leqslant r_0. \tag{3.15}$$

Introducing the irregular solution $G_\lambda(r)$ associated with Eq. (3.2) by[37]

$$G_\lambda(r) = F_\lambda(r)\int_r^{r_0} dr'\,[F_\lambda(r')]^{-2}, \tag{3.16}$$

we obtain the bound

$$|G_\lambda(r)| \leqslant c_2(r_0)^{-2} c_1(r_0) r^\lambda \int_r^{r_0} dr'\, r'^{-2\lambda}$$
$$\leqslant c_3(r_0)\begin{cases} r^{1/2}|\ln r|, & \lambda = \frac{1}{2}, \\ r^{1-\lambda}, & \frac{1}{2} < \lambda < \frac{3}{2}; \quad r \leqslant r_0. \end{cases} \tag{3.17}$$

We also note that $[G_\lambda, F_\lambda]_r = 1$.

Given the above preliminaries we now derive all self-adjoint extensions of h. The adjoint operator of h reads

$$h^* = -\frac{d^2}{dr^2} + \lambda(\lambda-1)r^{-2} + V,$$
$$\mathscr{D}(h^*) = \{ g \in L^2((0,\infty)) | g, g' AC_{\rm loc}((0,\infty)), \tag{3.18}$$
$$-g'' + \lambda(\lambda-1)r^{-2}g + Vg \in L^2((0,\infty))\},$$

and by the general theory of second-order ordinary differential operators all self-adjoint extensions h_ν of h are given by[30–32,38]

$$h_\nu = -\frac{d^2}{dr^2} + \lambda(\lambda-1)r^{-2} + V,$$
$$\mathscr{D}(h_\nu) = \{ g \in \mathscr{D}(h^*) | \lim_{r\to 0_+} [\phi_{\nu,\lambda}, g]_r = 0\},$$
$$-\infty < \nu \leqslant \infty, \tag{3.19}$$

where

$$\phi_{\nu,\lambda}(r) = G_\lambda(r) + \nu F_\lambda(r), \quad -\infty < \nu \leqslant \infty \tag{3.20}$$

[i.e., $\phi_{\infty,\lambda}(r) = F_\lambda(r)$ for $\nu = \infty$]. Since any $g \in \mathscr{D}(h^*)$ can be written as[38]

$$g(r) = c_1 F_\lambda(r) + c_2 G_\lambda(r) - F_\lambda(r)\int_\rho^r dr'\, G_\lambda(r')(h^*g)(r')$$
$$+ G_\lambda(r)\int_\rho^r dr'\, F_\lambda(r')(h^*g)(r'), \tag{3.21}$$

for some $\rho > 0$,

a straightforward computation shows

$$[\phi_{\nu,\lambda}, g]_r = c_1 - c_2\nu - \nu\int_\rho^r dr'\, F_\lambda(r')(h^*g)(r')$$
$$-\int_\rho^r dr'\, G_\lambda(r')(h^*g)(r'). \tag{3.22}$$

Thus we obtain for $g \in \mathscr{D}(h_\nu)$

$$c_1 - \int_\rho^r dr'\, G_\lambda(r')(h^*g)(r')$$
$$= \nu\left[c_2 + \int_\rho^r dr'\, F_\lambda(r')(h^*g)(r')\right]. \tag{3.23}$$

From Eqs. (3.12) and (3.14) we get

$$\lim_{r\to 0_+} F_\lambda(r)/G_\lambda^{(0)}(r) = 0, \quad \lim_{r\to 0_+} F_\lambda(r)/F_\lambda^{(0)}(r) = 1,$$
$$\widetilde{F}_\lambda(r) \underset{r\to 0_+}{=} o(1), \tag{3.24}$$

where

$$\widetilde{F}_\lambda(r) = -1 + [1 + \widehat{F}_\lambda(r)]^{-1}. \tag{3.25}$$

Thus Eq. (3.16) implies

$$G_\lambda(r) = F_\lambda^{(0)}(r)(1+\widehat{F}_\lambda(r))\int_r^{r_0} dr'(F_\lambda^{(0)}(r'))^{-2}(1+\widetilde{F}_\lambda(r'))^2$$
$$\underset{r\to 0_+}{=} G_\lambda^{(0)}(r) + o(G_\lambda^{(0)}(r)) \tag{3.26}$$

and hence

$$\lim_{r\to 0_+} G_\lambda(r)/G_\lambda^{(0)}(r) = 1. \tag{3.27}$$

Equations (3.24) and (3.27) together with Eq. (3.21) then prove

$$g_{0,\lambda} := \lim_{r\to 0_+} g(r)/G_\lambda^{(0)}(r)$$
$$= c_2 - \int_0^\rho dr'\, F_\lambda(r')(h^*g)(r'), \quad g \in \mathscr{D}(h^*). \tag{3.28}$$

If we insert the asymptotic expansion of $F_\lambda(r)$ as $r\to 0_+$ into Eq. (3.16) we get the corresponding expansion for $G_\lambda(r)$. Let $G_\lambda^B(r)$ denote the asymptotic expansion of $G_\lambda(r)$ up to the smallest order such that

$$\lim_{r\to 0_+} [G_\lambda(r) - G_\lambda^B(r)]/F_\lambda^{(0)}(r) = 0. \tag{3.29}$$

[A constructive approach to calculate $G_\lambda^B(r)$ will be given later on.] Then Eq. (3.21) implies

$$\frac{g(r)}{F_\lambda^{(0)}(r)} - g_{0,\lambda}\frac{G_\lambda^B(r)}{F_\lambda^{(0)}(r)}$$
$$= c_1\frac{F_\lambda(r)}{F_\lambda^{(0)}(r)} + c_2\frac{G_\lambda(r) - G_\lambda^B(r)}{F_\lambda^{(0)}(r)}$$
$$+ \frac{F_\lambda(r)}{F_\lambda^{(0)}(r)}\int_r^\rho dr'\, G_\lambda(r')(h^*g)(r')$$
$$- \frac{G_\lambda(r) - G_\lambda^B(r)}{F_\lambda^{(0)}(r)}\int_r^\rho dr'\, F_\lambda(r')(h^*g)(r')$$
$$+ \frac{G_\lambda^B(r)}{F_\lambda^{(0)}(r)}\int_0^r dr'\, F_\lambda(r')(h^*g)(r'). \tag{3.30}$$

Using Eqs. (3.15) and (3.17), one shows that

$$\left|\frac{G_\lambda^B(r)}{F_\lambda^{(0)}(r)}\int_0^r dr'\, F_\lambda(r')(h^*g)(r')\right|$$
$$\leqslant c_2(r_0)\begin{Bmatrix} r^{1/2}|\ln r|, & \lambda = \frac{1}{2} \\ r^{1-\lambda}, & \frac{1}{2} < \lambda < \frac{3}{2} \end{Bmatrix} r^{-\lambda}$$
$$\times\left(\int_0^r dr'|F_\lambda(r')|^2\right)^{1/2}\|h^*g\|_2$$
$$\leqslant \text{const}\begin{cases} r|\ln r|, & \lambda = \frac{1}{2}, \\ r^{3/2-\lambda}, & \frac{1}{2} < \lambda < \frac{3}{2}; \quad r \leqslant r_0. \end{cases} \tag{3.31}$$

Thus, we define

$$g_{1,\lambda} := \lim_{r\to 0_+} [g(r) - g_{0,\lambda}G_\lambda^B(r)]/F_\lambda^{(0)}(r), \quad g \in \mathscr{D}(h^*), \tag{3.32}$$

and obtain from Eqs. (3.30), (3.31), and the fact that h is in the limit circle case at the origin [i.e., $F_\lambda, G_\lambda \in L^2((0,R))$ for any $0<R<\infty$]

$$g_{1,\lambda} = c_1 + \int_0^\rho dr'\, G_\lambda(r')(h^* g)(r'), \quad g \in \mathscr{D}(h^*). \tag{3.33}$$

The self-adjoint boundary condition (3.23) thus reads

$$\nu g_{0,\lambda} = g_{1,\lambda}, \quad -\infty < \nu \leqslant \infty. \tag{3.34}$$

It is not hard to see that $\nu = \infty$, i.e., $g_{0,\lambda} = 0$ corresponds to the Friedrichs extension of h. For $|\nu| < \infty$, h_ν describes a $\lambda(\lambda-1)r^{-2} + \gamma r^{-1} + \alpha r^{-a} + W +$ "point interaction."

It remains to determine $G_\lambda^B(r)$ explicitly. Since W has no influence on boundary conditions we simply put $W=0$ from now on. As $G_\lambda^B(r)$ will be constructed with the help of Eq. (3.16), we first derive the asymptotic expansion of $F_\lambda(r)$ as $r \to 0_+$.

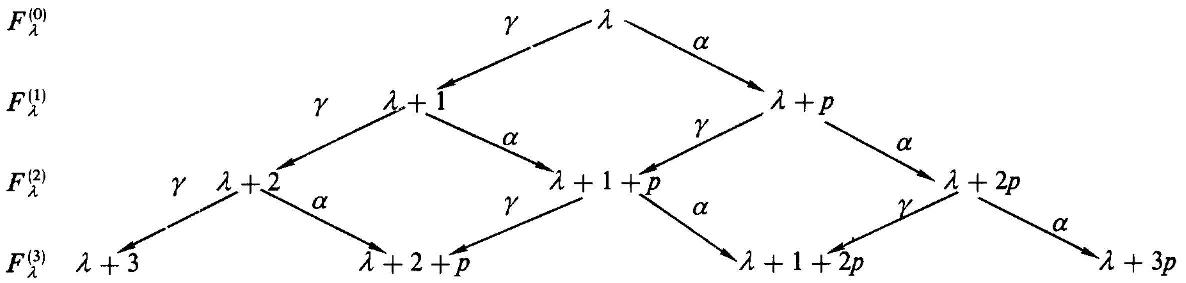
Suppose first that $\alpha = 0$ [i.e., $V(r) = \gamma r^{-1}$]. Then the mth iteration of Eq. (3.4) yields

$$F_{\lambda,\gamma}^{(m)}(r) = \left[m! \prod_{j=0}^{m-1} (2\lambda + j)\right]^{-1} \gamma^m r^{\lambda+m}, \quad m = 0,1,\ldots. \tag{3.35}$$

Similarly, if $\gamma = 0$ [i.e., $V(r) = \alpha r^{-a}$] the mth iteration of Eq. (3.4) yields

$$F_{\lambda,\alpha}^{(m)}(r) = \left[m!\, p^m \prod_{j=1}^{m} (2\lambda - 1 + jp)\right]^{-1} \alpha^m r^{\lambda+mp},$$
$$p = 2 - a, \quad m = 0,1,\ldots. \tag{3.36}$$

For the total potential $V(r) = \gamma r^{-1} + \alpha r^{-a}$ we get of course additional mixed exponents which are exhibited in the following diagram:



. (3.37)

After inserting the above asymptotic expansion of $F_\lambda(r)$ as $r \to 0_+$ into Eq. (3.16) a closer look at condition (3.29) and (3.16) then shows that in order to obtain $G_\lambda^B(r)$ we need an asymptotic expansion for $F_\lambda(r)$ up to exponents of the type r^s, $s \leqslant 3\lambda - 1$. We denote the corresponding asymptotic expansion of $F_\lambda(r)$ by $F_\lambda^B(r)$, i.e.,

$$F_\lambda(r) - F_\lambda^B(r) \underset{r\to 0_+}{=} o(r^s), \quad s \leqslant 3\lambda - 1. \tag{3.38}$$

Using Eq. (3.16) this implies that $G_\lambda^B(r)$ represents the asymptotic expansion of $G_\lambda(r)$ as $r \to 0_+$ up to the order r^t, $t \leqslant 2\lambda - 1$, i.e.,

$$G_\lambda(r) - G_\lambda^B(r) \underset{r\to 0_+}{=} o(r^t), \quad t \leqslant 2\lambda - 1. \tag{3.39}$$

The above-described mechanism works for all $\frac{1}{2} \leqslant \lambda < \frac{3}{2}$, $\gamma \in \mathbb{R}$ and $0 < a < 2$. But clearly the number of terms in $F_\lambda^B(r)$ and $G_\lambda^B(r)$ drastically increases as $a \to 2_-$ as long as λ runs through the whole interval $-\frac{1}{2} \leqslant \lambda < \frac{3}{2}$. In order to keep the treatment reasonably short we give a complete discussion in the case $p \geqslant \frac{1}{2}$ (i.e., $0 < a \leqslant \frac{3}{2}$). From diagram (3.37) and (3.38) we infer that $F_\lambda^B(r)$ must consist of the terms r^λ, $r^{\lambda+p}$, $r^{\lambda+1}$, $r^{\lambda+2p}$, $r^{\lambda+1+p}$, and $r^{\lambda+3p}$. More precisely

$$F_\lambda^B(r) = r^\lambda [1 + A_1 r^p + (\gamma/2\lambda) r + A_2 r^{2p} + A_3 r^{3p} + A_4 r^{1+p}], \tag{3.40}$$

$$\begin{aligned} A_1 &= [p(2\lambda + p - 1)]^{-1}\alpha, \\ A_2 &= [2p^2(2\lambda + p - 1)(2\lambda + 2p - 1)]^{-1}\alpha^2, \\ A_3 &= [6p^3(2\lambda + p - 1)(2\lambda + 2p - 1)(2\lambda + 3p - 1)]^{-1}\alpha^3, \\ A_4 &= (p+1)^{-1}(2\lambda + p)^{-1}\{[p(2\lambda + p - 1)]^{-1} - (2\lambda)^{-1}\}\gamma\alpha. \end{aligned} \tag{3.41}$$

Next we compute $G_\lambda^B(r)$. By Eq. (3.39) we have to take into account terms up to order r^{3p}. According to Eq. (3.16) we expand

$$F_\lambda^B(r) \int_r^{r_0} dr'\, r'^{-2\lambda} [1 + f^B(r')]^{-1}, \tag{3.42}$$

where

$$\begin{aligned} [F_\lambda^B(r)]^2 &= r^{2\lambda}[1 + f^B(r)], \\ f^B(r) &= 2A_1 r^p + (\gamma/\lambda) r + (2A_2 + A_1^2) r^{2p} \\ &\quad + [2A_4 + (A_1\gamma/\lambda)] r^{1+p} + (2A_3 + 2A_1A_2) r^{3p}. \end{aligned} \tag{3.43}$$

Taking r_0 small enough $(0 < r \leqslant r_0)$ we get $|f^B(r)| < 1$ for $r \in [0, r_0]$ and hence

$$\begin{aligned} [1 + f^B(r)]^{-1} \underset{r\to 0_+}{=} & 1 - 2A_1 r^p + (3A_1^2 - 2A_2) r^{2p} \\ & - (\gamma/\lambda) r + (6A_1A_2 - 4A_1^3 - 2A_3) r^{3p} \\ & + [(3A_1\gamma/\lambda) - 2A_4] r^{1+p} + O(r^{1+2p}). \end{aligned} \tag{3.44}$$

A formal integration then yields

$$\begin{aligned} \int_r^{r_0} & dr'\, r'^{-2\lambda} [1 + f^B(r')]^{-1} \\ &= r^{1-2\lambda} \left\{ \frac{1}{2\lambda - 1} + 2A_1 \frac{r^p}{p + 1 - 2\lambda} + (2A_2 - 3A_1^2) \right. \\ &\quad \times \frac{r^{2p}}{2p + 1 - 2\lambda} + \frac{\gamma}{\lambda} \frac{r}{2(1-\lambda)} \\ &\quad + (4A_1^3 + 2A_4 - 6A_1A_2) \end{aligned}$$

$$\times \frac{r^{3p}}{3p+1-2\lambda} + [2A_3 - (3A_1\gamma/\lambda)] \frac{r^{1+p}}{2(1-\lambda)+p} + C(r_0) + O(r^{1+2p}) \Bigg\} . \quad (3.45)$$

But Eq. (3.45) has to be supplemented by the following exceptions:

If $\lambda = \frac{1}{2}$,

$\frac{r^{1-2\lambda}}{2\lambda - 1}$ should be replaced by $(-\ln r)$;

if $\lambda = 1$,

$\frac{r^{2(1-\lambda)}}{2(1-\lambda)}$ should be replaced by $\ln r$;

if $p = 2\lambda - 1$,

$\frac{r^{p+1-2\lambda}}{p+1-2\lambda}$ should be replaced by $\ln r$;

(3.46)

if $p = (2\lambda - 1)/2$,

$\frac{r^{2p+1-2\lambda}}{2p+1-2\lambda}$ should be replaced by $\ln r$;

if $p = (2\lambda - 1)/3$,

$\frac{r^{3p+1-2\lambda}}{3p+1-2\lambda}$ should be replaced by $\ln r$

if $p = 2(\lambda - 1)$,

$\frac{r^{2(1-\lambda)+p}}{2(1-\lambda)+p}$ should be replaced by $\ln r$.

Without loss of generality we take $C(r_0) = 0$ and obtain from Eqs. (3.16) and (3.45)

$$G^B_\lambda(r) = G^{(0)}_\lambda(r) + r^{1-\lambda}\{B_1 r^p + B_2 r^{2p} - \gamma[2(1-2\lambda)(1-\lambda)]^{-1} r + B_3 r^{3p} + B_4 r^{1+p}\}, \quad (3.47)$$

$$B_1 = [2(p+1-2\lambda)^{-1} + (2\lambda-1)^{-1}]A_1,$$
$$B_2 = (p+1-2\lambda)^{-1} 2A_1^2 + (2p+1-2\lambda)^{-1} \times [2A_2 - 3A_1^2] + (2\lambda-1)^{-1}A_2, \quad (3.48)$$
$$B_3 = (3p+1-2\lambda)^{-1}(4A_1^3 + 2A_3 - 6A_1A_2) + (2p+1-2\lambda)^{-1}(2A_1A_2 - 3A_1^3) + (p+1-2\lambda)^{-1}2A_1A_2 + (2\lambda-1)^{-1}A_3,$$
$$B_4 = \{[\lambda(p+1-2\lambda)]^{-1} + [2\lambda(1-\lambda)]^{-1}\}\gamma A_1 + [2(1-\lambda)+p]^{-1}[2A_4 - (3\gamma A_1/\lambda)] + (2\lambda-1)^{-1}A_4.$$

Of course Eqs. (3.47) and (3.48) do not hold for the exceptional values of λ and p [listed in (3.46)]. If λ takes on some of the values described in (3.46) then $G^B_\lambda(r)$ results after inserting the corresponding logarithmic term in Eq. (3.45) and multiplying with $F^B_\lambda(r)$. These logarithmic cases are familiar from the theory of Fuchsian differential equations.

Finally, we note two special cases.

(A) $\lambda = \frac{1}{2}$ (the s-wave Schrödinger operator in two dimensions): In this case the construction of $F^B_{1/2}(r)$ and $G^B_{1/2}(r)$ is particularly simple since Eqs. (3.38) and (3.39) imply

$$F^B_{1/2}(r) = F^{(0)}_{1/2}(r) = r^{1/2}, \qquad G^B_{1/2}(r) = G^{(0)}_{1/2}(r) = -r^{1/2}\ln r, \quad (3.49)$$

and thus

$$g_{0,1/2} = \lim_{r\to 0_+} [-(r^{1/2}\ln r)^{-1} g(r)], \qquad g_{1,1/2} = \lim_{r\to 0_+} r^{-1/2}[g(r) + g_{0,1/2} r^{1/2}\ln r], \quad g \in \mathscr{D}(h^*). \quad (3.50)$$

(B) $\lambda = 1$ (the s-wave Schrödinger operator in three dimensions): For $p > \frac{1}{4}$ (i.e., $0 < a < \frac{7}{4}$) one obtains

$$G^B_1(r) = 1 + B'_1 r^p + B'_2 r^{2p} + \gamma r \ln r + (\gamma/2) r + B'_3 r^{3p}, \quad (3.51)$$

$$B'_1 = [1 + (p-1)^{-1}2]A'_1,$$
$$B'_2 = A'_2 + (p-1)^{-1}2A'^2_1 + (2p-1)^{-1}(2A'_2 - 3A'^2_1), \quad (3.52)$$
$$B'_3 = A'_3 + (3p+1-2)^{-1}(4A'^3_1 + 2A'_3 - 6A'_1A'_2) + (p-1)^{-1}2A'_1A'_2 + (2p-1)^{-1}(2A'_1A'_2 - 3A'^2_1),$$

and

$$A'_1 = [p(p+1)]^{-1}\alpha, \quad A'_2 = [2p^2(p+1)(2p+1)]^{-1}\alpha^2, \quad A'_3 = [6p^3(p+1)(2p+1)(3p+1)]^{-1}\alpha^3. \quad (3.53)$$

For $p > \frac{1}{3}$ one can delete the r^{3p} term and for $p > \frac{1}{2}$ one can in addition delete the r^{2p} term in Eq. (3.51).

Summarizing the whole section, we have proved the following.

Theorem 3.1: Assume the conditions in (3.1). Then all self-adjoint extensions h_ν of h can be characterized by

$$h_\nu = -\frac{d^2}{dr^2} + \lambda(\lambda-1)r^{-2} + \gamma r^{-1} + \alpha r^{-a} + W,$$
$$\mathscr{D}(h_\nu) = \{g \in L^2((0,\infty)) | g, g' \in AC_{\text{loc}}((0,\infty)); \ \nu g_{0,\lambda} = g_{1,\lambda}; \ -g'' + \lambda(\lambda-1)r^{-2}g + \gamma r^{-1}g + \alpha r^{-a}g \in L^2((0,\infty))\}, \quad (3.54)$$
$$-\infty < \nu \leqslant \infty, \quad \tfrac{1}{2} \leqslant \lambda < \tfrac{3}{2}, \quad \alpha, \gamma \in \mathbb{R}, \quad 0 < a < 2.$$

Here the boundary values $g_{0,\lambda}$ and $g_{1,\lambda}$ are defined as

$$g_{0,\lambda} = \lim_{r\to 0_+} g(r)/G^{(0)}_\lambda(r), \qquad g_{1,\lambda} = \lim_{r\to 0_+} [g(r) - g_{0,\lambda} G^B_\lambda(r)]/F^{(0)}_\lambda(r), \quad g \in \mathscr{D}(h^*), \quad (3.55)$$

where $F^{(0)}_\lambda(r)$ and $G^{(0)}_\lambda(r)$ are given by Eq. (3.6) and $G^B_\lambda(r)$ denotes the asymptotic expansion of $G_\lambda(r)$ as $r \to 0_+$ up to order r^t, $t \leqslant 2\lambda - 1$. The boundary condition $g_{0,\lambda} = 0$ (i.e., $\nu = \infty$) represents the Friedrichs extension of h.

In the trivial case $\lambda = 1$, $\alpha = \gamma = 0$, the boundary values take on the familiar form

$$g_{0,1} = g(0_+), \quad g_{1,1} = g'(0_+). \tag{3.56}$$

Remark 3.2: In the special case where $V(r)$ has a Laurent expansion of the type $V(r) = \Sigma_{m=-2}^{\infty} a_m r^m$ near the origin, the above result has been derived by Rellich.[13] His proof relies entirely on the meromorphic structure of V whereas ours seems to be more direct and covers the general case $V(r) = \alpha r^{-a}, 0 < a < 2$. It is obvious from the arguments presented above that our method extends to potentials of the type

$$V(r) = \sum_{j=1}^{N} \alpha_j r^{-a_j} + W,$$
$$W \in L^{\infty}((0,\infty)) \text{ real valued}, \quad \alpha_j \in \mathbb{R},$$
$$0 < a_j < 2, \quad N \in \mathbb{N}. \tag{3.57}$$

In addition, our analysis extends in a straightforward manner to $\lambda(\lambda - 1) \in \mathbb{R}$ since semiboundedness of h (i.e., $\lambda \geqslant \frac{1}{2}$) turns out to be inessential.

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