Chapter 8

The spectral shift function: Abstract facts

The significance of Theorem 7.4 is that the trace class condition (7.10) permits one to define a spectral shift function for the pair (H, H_0). To make this precise, we introduce the class of functions $\mathfrak{F}_r(\mathbb{R})$, $r \in \mathbb{N}$, by

$$\mathfrak{F}_r(\mathbb{R}) := \big\{ f \in C^2(\mathbb{R}) \,\big|\, f^{(\ell)} \in L^\infty(\mathbb{R});\ \text{there exists } \varepsilon > 0 \text{ and } f_0 = f_0(f) \in \mathbb{C} \\ \text{such that } (d^\ell/d\lambda^\ell)\big[f(\lambda) - f_0\lambda^{-r}\big] \underset{|\lambda|\to\infty}{=} O\big(|\lambda|^{-\ell-r-\varepsilon}\big),\ \ell = 0,1,2\big\}. \tag{8.1}$$

(It is implied that $f_0 = f_0(f)$ is the same as $\lambda \to \pm\infty$.) One observes that $C_0^\infty(\mathbb{R}) \subset \mathfrak{F}_r(\mathbb{R})$, $r \in \mathbb{N}$.

In [111], M. Krein established the existence of a spectral shift function corresponding to any pair of resolvent comparable self-adjoint operators. Specifically, Krein proved that if S_0 and S are self-adjoint and satisfy

$$\big[(S - zI_{\mathcal{H}})^{-1} - (S_0 - zI_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}) \tag{8.2}$$

for some (and, hence, for all) $z \in \mathbb{C}\backslash\mathbb{R}$, then

$$\big[f(S) - f(S_0)\big] \in \mathcal{B}_1(\mathcal{H}), \quad f \in \mathfrak{F}_1(\mathbb{R}),$$

and there exists a real-valued spectral shift function

$$\xi(\,\cdot\,; S, S_0) \in L^1\big(\mathbb{R}, \big(1 + |\lambda|\big)^{-2}\, d\lambda\big)$$

so that

$$\operatorname{tr}_{\mathcal{H}}\big(f(S) - f(S_0)\big) = \int_{\mathbb{R}} \xi(\lambda; S, S_0) d\lambda\, f'(\lambda), \quad f \in \mathfrak{F}_1(\mathbb{R}). \tag{8.3}$$

One limitation to Krein's theory is that the condition (8.2) generally does not hold for Schrödinger operators in dimensions $n \geq 4$. Similar difficulties are encountered for the polyharmonic operator (cf. [186, Section 3.4]) and the Dirac operator (cf. [186, Section 3.5.3] and Theorem 7.4). In these cases, only the difference of higher powers of the resolvents belongs to the trace class (cf. [186, Remark 3.3.3]). Using the theory of double operator integrals, Yafaev [185] proved the existence of a spectral shift function under the weaker assumption that the difference of an odd power of the resolvents belongs to the trace class.

Theorem 8.1 ([185, Theorem 2.2]). *Let $r \in \mathbb{N}$, r odd, and suppose that S_0 and S are self-adjoint operators in $\mathcal{H}$ with*

$$\big[(S - zI_{\mathcal{H}})^{-r} - (S_0 - zI_{\mathcal{H}})^{-r}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{8.4}$$

Then

$$\big[f(S) - f(S_0)\big] \in \mathcal{B}_1(\mathcal{H}), \quad f \in \mathfrak{F}_r(\mathbb{R}),$$

and there exists a function

$$\xi(\,\cdot\,; S, S_0) \in L^1\big(\mathbb{R}; \big(1 + |\lambda|\big)^{-r-1}\, d\lambda\big) \tag{8.5}$$

such that the following trace formula holds,

$$\operatorname{tr}_{\mathcal{H}}\big(f(S) - f(S_0)\big) = \int_{\mathbb{R}} \xi(\lambda; S, S_0) d\lambda\, f'(\lambda), \quad f \in \mathfrak{F}_r(\mathbb{R}).$$

In particular, one has

$$\operatorname{tr}_{\mathcal{H}}\big((S - zI_{\mathcal{H}})^{-r} - (S_0 - zI_{\mathcal{H}})^{-r}\big) = -r \int_{\mathbb{R}} \frac{\xi(\lambda; S, S_0) d\lambda}{(\lambda - z)^{r+1}}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{8.6}$$

Remark 8.2. The above theorem, together with Theorem 7.4 guarantees that for Dirac operators H and H_0 in $[L^2(\mathbb{R}^n)]^N$ the spectral shift function $\xi(\,\cdot\,; H, H_0)$ exists. However, for the representation of the spectral shift function in terms of a regularized perturbation determinant it is desirable to take the regularized determinant $\det_{\mathcal{H},p}((H - zI_{\mathcal{H}})(H_0 - zI_{\mathcal{H}})^{-1})$ with p equal to $n + 1$. Theorem 8.1 permits this in odd space dimensions n. In even space dimensions Theorem 8.1 does not guarantee the appropriate integrability of the spectral shift function $\xi(\,\cdot\,; H, H_0)$ and so one would be forced to consider a regularized determinant with $p = n + 2$. To avoid this drawback, we prove that under a certain stronger condition (satisfied for Dirac operators H and H_0 considered in Chapter 3) an analogue of Theorem 8.1 holds for any $r \in \mathbb{N}$. ◇

Hypothesis 8.3. *Let $r \in \mathbb{N}$ and assume that S and S_0 are self-adjoint operators in $\mathcal{H}$ with a common dense domain, such that*

$$(S - S_0) \in \mathcal{B}(\mathcal{H}),$$

and for some $0 < \varepsilon < 1/2$,

$$(S - S_0)(S_0^2 + I_{\mathcal{H}})^{-(r/2)-\varepsilon} \in \mathcal{B}_1(\mathcal{H}). \tag{8.7}$$

Remark 8.4. (i) Assuming Hypothesis 8.3, it follows that

$$(S - S_0)(S_0 - zI_{\mathcal{H}})^{-r-1} \in \mathcal{B}_1(\mathcal{H}).$$

Since $(S - S_0) \in \mathcal{B}(\mathcal{H})$, it follows from the three line theorem that

$$(S - S_0)(S_0 - zI_{\mathcal{H}})^{-j} \in \mathcal{B}_{(r+1)/j}(\mathcal{H}), \quad j \in \mathbb{N},\ 1 \leq j \leq r + 1. \tag{8.8}$$

Furthermore, another application of the three line theorem implies

$$(S_0 - zI_{\mathcal{H}})^{-j_1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-j_2} \in \mathcal{B}_{(r+1)/(j_1+j_2)}(\mathcal{H}) \tag{8.9}$$

for all $j_1, j_2 \in \mathbb{N}$, with $1 \leq j_1 + j_2 \leq r + 1$.

(ii) For the proof of Theorem 8.12 we will only need (8.7) and (8.8). We assumed boundedness of $S - S_0$ only to get (8.8) as a consequence of (8.7). It is possible to go beyond this boundedness assumption, but we omit further details at this point.

(iii) The inclusion (7.15) shows that assumption (8.7) holds with $r = n$ for the pair of Dirac operators (H, H_0) as long as V satisfies Hypothesis 7.1. ◇

The following result appeared in [44, Theorem 2.7].

Theorem 8.5. *Assume Hypothesis 8.3. For any $j = 1, \dots, r$, one has*

$$(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j} \in \mathcal{B}_{(r+1)/(j+1)}(\mathcal{H}).$$

Lemma 8.6. *Assume Hypothesis 8.3. For any $j = 1, \dots, r$, and $z \in \mathbb{C}\backslash\mathbb{R}$, one has*

$$\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S_0 + zI_{\mathcal{H}})^{-r+j} \in \mathcal{B}_1(\mathcal{H}).$$

Proof. We prove the claim by induction on j. Let $j = 1$. Using the resolvent identity twice one writes

$$\begin{aligned}
&\big[(S - zI_{\mathcal{H}})^{-1} - (S_0 - zI_{\mathcal{H}})^{-1}\big](S_0 + zI_{\mathcal{H}})^{-r+1} \\
&= -(S - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+1} \\
&= (S - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+1} \\
&\quad - (S_0 - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+1}.
\end{aligned} \tag{8.10}$$

By (8.9) one obtains

$$(S_0 - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-r} \in \mathcal{B}_1(\mathcal{H}),$$

and therefore the second term on the right-hand side of (8.10) is a trace-class operator. By (8.8),

$$\begin{aligned}
(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1} &\in \mathcal{B}_{r+1}(\mathcal{H}), \\
(S - S_0)(S_0 - zI_{\mathcal{H}})^{-r} &\in \mathcal{B}_{(r+1)/r}(\mathcal{H}),
\end{aligned}$$

guaranteeing that the first term on the right-hand side of (8.10) is also a trace-class operator. Thus, one concludes that

$$\big[(S - zI_{\mathcal{H}})^{-1} - (S_0 - zI_{\mathcal{H}})^{-1}\big](S_0 + zI_{\mathcal{H}})^{-r+1} \in \mathcal{B}_1(\mathcal{H}),$$

proving the first induction step.

Next, suppose that

$$\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S_0 + zI_{\mathcal{H}})^{-r+j} \in \mathcal{B}_1(\mathcal{H})$$

for some $j = 1, \dots r-1$. Writing

$$\begin{aligned}
&\big[(S - zI_{\mathcal{H}})^{-j-1} - (S_0 - zI_{\mathcal{H}})^{-j-1}\big](S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\quad = \big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\qquad + (S_0 - zI_{\mathcal{H}})^{-j}\big[(S - zI_{\mathcal{H}})^{-1} - (S_0 - zI_{\mathcal{H}})^{-1}\big](S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\quad := (I) + (II),
\end{aligned} \tag{8.11}$$

we will treat the terms (I) and (II) separately in the following.

For (I) on the right-hand side of (8.11) one gets

$$\begin{aligned}
&\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\quad = \big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big] \\
&\qquad \times \big[(S - zI_{\mathcal{H}})^{-1} - (S_0 - zI_{\mathcal{H}})^{-1}\big](S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\qquad + \big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\quad = -\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S - zI_{\mathcal{H}})^{-1} \\
&\qquad \times (S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\qquad + \big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1}.
\end{aligned}$$

By the induction hypothesis one concludes that

$$\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S_0 + zI_{\mathcal{H}})^{-r+j} \in \mathcal{B}_1(\mathcal{H}),$$

and therefore also

$$\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1} \in \mathcal{B}_1(\mathcal{H}).$$

By Theorem 8.5 one obtains

$$\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big] \in \mathcal{B}_{(r+1)/(j+1)}(\mathcal{H}),$$

and by (8.8),

$$(S - S_0)(S_0 + zI_{\mathcal{H}})^{-r+j} \in \mathcal{B}_{(r+1)/(r-j)}(\mathcal{H}).$$

Therefore,

$$\begin{aligned}
&\big[(S - zI_{\mathcal{H}})^{-j} - (S_0 - zI_{\mathcal{H}})^{-j}\big](S - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1} \\
&\quad \times (S_0 + zI_{\mathcal{H}})^{-r+j+1} \in \mathcal{B}_{(r+1)/(j+1)}(\mathcal{H}) \cdot \mathcal{B}_{(r+1)/(r-j)}(\mathcal{H}) \subset \mathcal{B}_1(\mathcal{H}), \\
&\hspace{20em} 1 \leq j \leq r-1.
\end{aligned}$$

Thus, $(I) \in \mathcal{B}_1(\mathcal{H})$.

To show that also (II) on the right-hand side of (8.11) is a trace-class operator, one writes

$$
\begin{aligned}
&(S_0 - zI_{\mathcal{H}})^{-j}\big[(S - zI_{\mathcal{H}})^{-1} - (S_0 - zI_{\mathcal{H}})^{-1}\big](S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&= -(S_0 - zI_{\mathcal{H}})^{-j}(S - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&= -(S_0 - zI_{\mathcal{H}})^{-j}(S_0 - zI_{\mathcal{H}})^{-1}(S - S_0)(S - zI_{\mathcal{H}})^{-1} \\
&\quad \times (S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1} \\
&\quad + (S_0 - zI_{\mathcal{H}})^{-j}(S_0 - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}(S_0 + zI_{\mathcal{H}})^{-r+j+1}.
\end{aligned}
$$

By (8.8) one infers

$$
\begin{aligned}
(S_0 - zI_{\mathcal{H}})^{-j-1}(S - S_0) &\in \mathcal{B}_{(r+1)/(j+1)}(\mathcal{H}), \\
(S - S_0)(S_0 + zI_{\mathcal{H}})^{-r+j} &\in \mathcal{B}_{(r+1)/(r-j)}(\mathcal{H}),
\end{aligned}
$$

and hence,

$$
\begin{aligned}
&(S_0 - zI_{\mathcal{H}})^{-j}(S_0 - zI_{\mathcal{H}})^{-1}(S - S_0)(S - zI_{\mathcal{H}})^{-1}(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1} \\
&\quad \times (S_0 + zI_{\mathcal{H}})^{-r+j+1} \in \mathcal{B}_1(\mathcal{H}).
\end{aligned}
$$

Furthermore, by (8.9),

$$
(S_0 + zI_{\mathcal{H}})^{-j-1}(S - S_0)(S_0 + zI_{\mathcal{H}})^{-r+j} \in \mathcal{B}_1(\mathcal{H}), \quad 1 \leq j \leq r - 1.
$$

Thus, also (II) is a trace-class operator. Combining this with the fact that $(I) \in \mathcal{B}_1(\mathcal{H})$ and referring to (8.11), one concludes that

$$
\big[(S - zI_{\mathcal{H}})^{-j-1} - (S_0 - zI_{\mathcal{H}})^{-j-1}\big](S_0 + zI_{\mathcal{H}})^{-r+j+1} \in \mathcal{B}_1(\mathcal{H}). \qquad \blacksquare
$$

From this point on we assume Hypothesis 8.3 for even $r = 2k$ for the remainder of this chapter. Introducing the function

$$
\phi(t) = t(1 + t^2)^{(r-1)/2} = t(1 + t^2)^{k-(1/2)}, \quad t \in \mathbb{R}, \tag{8.12}
$$

we aim at proving that

$$
\big[(\phi(S) + iI_{\mathcal{H}})^{-1} - (\phi(S_0) + iI_{\mathcal{H}})^{-1}\big] \in \mathcal{B}_1(\mathcal{H}), \tag{8.13}
$$

guaranteeing that the spectral shift function $\xi(\,\cdot\,; \phi(S), \psi(S_0))$ is well defined. Since

$$
\phi'(t) = (1 + t^2)^{(m-3)/2}(1 + rt^2) \geq 1 > 0,
$$

it follows that ϕ is a strictly monotone increasing function on $\mathbb{R}$. Therefore, one can use the invariance principle for the spectral shift function (see [184, Section 8.11]) to introduce $\xi(\,\cdot\,; S, S_0)$ by setting

$$
\xi(\lambda; S, S_0) = \xi\big(\phi(\lambda); \phi(S), \phi(S_0)\big) \quad \text{for a.e. } \lambda \in \mathbb{R}.
$$

The choice of ϕ and integrability properties of $\xi(\,\cdot\,;\phi(S),\phi(S_0))$ will imply an appropriate integrability condition for $\xi(\,\cdot\,;S,S_0)$.

A crucial result in the proof of the inclusion (8.13) is the following result. We recall that the Hölder space $C^{1,\alpha}([0,1])$, $0 \le \alpha \le 1$, is the class of functions f on $[0,1]$ such that

$$\|f\|_{C^{1,\alpha}([0,1])} = \|f\|_{C^1([0,1])} + \sup_{t_1,t_2\in[0,1]} \frac{|f'(t_1) - f'(t_2)|}{|t_1 - t_2|^\alpha} < \infty.$$

Theorem 8.7 ([135, Theorem 4 and Corollary 2]). *Suppose that A and B are self-adjoint operators on a Hilbert space $\mathcal{H}$, such that $(A - B) \in \mathcal{B}_1(\mathcal{H})$ and $\sigma(A) \cup \sigma(B) \subset [0,1]$. For any function $f \in C^{1,\alpha}([0,1])$ with $0 < \alpha \le 1$ one has*

$$\big[f(A) - f(B)\big] \in \mathcal{B}_1(\mathcal{H})$$

and

$$\big\|f(A) - f(B)\big\|_{\mathcal{B}_1(\mathcal{H})} \le C\|A - B\|_{\mathcal{B}_1(\mathcal{H})},$$

where the constant C is independent of A and B.

Assuming Hypothesis 8.3 with $r = 2k$, $k \in \mathbb{N}$, we intend to use Theorem 8.7 for the operators $A = (S^2 + I_{\mathcal{H}})^{-k}$ and $B = (S_0^2 + I_{\mathcal{H}})^{-k}$. In the following Lemma 8.8 we will show that with this choice of operators A, B the condition $(A - B) \in \mathcal{B}_1(\mathcal{H})$ of Theorem 8.7 is satisfied.

Lemma 8.8. *Assume Hypothesis 8.3 with $r = 2k$ for some $k \in \mathbb{N}$. Then*

$$\big[(S^2 + I_{\mathcal{H}})^{-k} - (S_0^2 + I_{\mathcal{H}})^{-k}\big] \in \mathcal{B}_1(\mathcal{H}).$$

Proof. One writes

$$\begin{aligned}
&(S^2 + I_{\mathcal{H}})^{-k} - (S_0^2 + I_{\mathcal{H}})^{-k} \\
&\quad = (S + iI_{\mathcal{H}})^{-k}(S - iI_{\mathcal{H}})^{-k} - (S_0 + iI_{\mathcal{H}})^{-k}(S_0 - iI_{\mathcal{H}})^{-k} \\
&\quad = \big[(S + iI_{\mathcal{H}})^{-k} - (S_0 + iI_{\mathcal{H}})^{-k}\big]\big[(S - iI_{\mathcal{H}})^{-k} - (S_0 - iI_{\mathcal{H}})^{-k}\big] \\
&\qquad + \big[(S + iI_{\mathcal{H}})^{-k} - (S_0 + iI_{\mathcal{H}})^{-k}\big](S_0 - iI_{\mathcal{H}})^{-k} \\
&\qquad + (S_0 + iI_{\mathcal{H}})^{-k}\big[(S - iI_{\mathcal{H}})^{-k} - (S_0 - iI_{\mathcal{H}})^{-k}\big]. \qquad (8.14)
\end{aligned}$$

By Lemma 8.6, the second and the third terms are trace-class operators. By Theorem 8.5 one infers that

$$\big[(S + iI_{\mathcal{H}})^{-k} - (S_0 + iI_{\mathcal{H}})^{-k}\big] \in \mathcal{B}_{(r+1)/(k+1)}(\mathcal{H}).$$

Therefore, the first term on the right-hand side of (8.14) is a trace-class operator too. ∎

Lemma 8.9. *Let $k \in \mathbb{N}$ and introduce the functions*

$$h_1(t) = \frac{1}{t^2(1+t^2)^{2k-1}+1}, \quad h_2(t) = \frac{(1+t^2)^k}{t^2(1+t^2)^{2k-1}+1}, \quad t \in \mathbb{R}.$$

There exist $f_1, f_2 \in C^{1,(1/k)}([0,1])$ such that

$$h_1(t) = f_1\big((1+t^2)^{-k}\big), \quad h_2(t) = f_2\big((1+t^2)^{-k}\big), \quad t \in \mathbb{R}.$$

Proof. We set

$$f_1(u) = \frac{u^2}{1-u^{1/k}+u^2}, \quad f_2(u) = \frac{u}{1-u^{1/k}+u^2}, \quad u \in [0,1].$$

A direct verification shows that

$$h_1(t) = f_1\big((1+t^2)^{-k}\big), \quad h_2(t) = f_2\big((1+t^2)^{-k}\big), \quad t \in \mathbb{R}.$$

Since

$$1-u^{1/k}+u^2 > 0, \quad u \in [0,1],$$

$f_1, f_2 \in C([0,1])$. By the fact $f_1(u) = uf_2(u)$, $u \in [0,1]$, it suffices to show that $f_2 \in C^{1,(1/k)}([0,1])$. One verifies that

$$\begin{aligned} f_2'(u) &= \frac{[1-u^{1/k}+u^2] - u[-\frac{1}{k}u^{(1/k)-1}+2u]}{[1-u^{1/k}+u^2]^2} \\ &= \frac{1-\big[1-(1/k)\big]u^{1/k}-u^2}{[1-u^{1/k}+u^2]^2}. \end{aligned}$$

Clearly $f_j \in C([0,1])$, $j = 1,2$. Furthermore, since the map $u \mapsto u^{1/k}$ is of Hölder class $C^{0,(1/k)}([0,1])$ and the map $u \mapsto \big[1-u^{1/k}+u^2\big]^{-2}$ is bounded on $[0,1]$, it follows that $f_2' \in C^{0,(1/k)}([0,1])$, that is, $f_2 \in C^{1,(1/k)}([0,1])$, as required. ∎

Lemma 8.10. *Assume Hypothesis 8.3 with $r = 2k$ for some $k \in \mathbb{N}$. Let h_2 be as in Lemma 8.9 and introduce*

$$g(t) = \frac{t}{(1+t^2)^{1/2}}, \quad t \in \mathbb{R}.$$

Then,

$$\big[g(S) - g(S_0)\big]h_2(S_0) \in \mathcal{B}_1(\mathcal{H}).$$

Proof. Since

$$h_2(t) = \frac{(1+t^2)^k}{t^2(1+t^2)^{2k-1}+1} \underset{|t|\to\infty}{=} O\big((1+t^2)^{-k}\big),$$

it suffices to show that

$$\big[g(S)-g(S_0)\big](S_0^2+I_{\mathcal{H}})^{-k}\in\mathcal{B}_1(\mathcal{H}).$$

By [38, Lemma 3.1],

$$\begin{aligned} &g(S)-g(S_0)\\ &\quad=\frac{1}{\pi}\operatorname{Re}\bigg(\int_0^\infty\frac{d\lambda}{\lambda^{1/2}}\Big[\big(S+i(\lambda+1)^{1/2}I_{\mathcal{H}}\big)^{-1}-\big(S_0+i(\lambda+1)^{1/2}I_{\mathcal{H}}\big)^{-1}\Big]\bigg),\end{aligned}$$

with a convergent Bochner integral in $\mathcal{B}(\mathcal{H})$. The substitution $\theta=(1+\lambda)^{1/2}$ then yields

$$g(S)-g(S_0)=\frac{1}{\pi}\operatorname{Re}\bigg(\int_1^\infty\frac{\theta d\theta}{(\theta^2-1)^{1/2}}\big[(S+i\theta I_{\mathcal{H}})^{-1}-(S_0+i\theta I_{\mathcal{H}})^{-1}\big]\bigg).$$

Therefore, it suffices to prove that

$$\int_1^\infty\frac{\theta d\theta}{(\theta^2-1)^{1/2}}\big[(S\pm i\theta I_{\mathcal{H}})^{-1}-(S_0\pm i\theta I_{\mathcal{H}})^{-1}\big](S_0^2+I_{\mathcal{H}})^{-k},$$

are convergent integrals in $\mathcal{B}_1(\mathcal{H})$.

The resolvent identity implies

$$\begin{aligned} &\int_1^\infty\frac{\theta d\theta}{(\theta^2-1)^{1/2}}\big[(S\pm i\theta I_{\mathcal{H}})^{-1}-(S_0\pm i\theta I_{\mathcal{H}})^{-1}\big]\big(S_0^2+I_{\mathcal{H}}\big)^{-k}\\ &\quad=-\int_1^\infty\frac{\theta d\theta}{(\theta^2-1)^{1/2}}(S\pm i\theta I_{\mathcal{H}})^{-1}(S-S_0)(S_0\pm i\theta I_{\mathcal{H}})^{-1}\big(S_0^2+I_{\mathcal{H}}\big)^{-k}.\end{aligned}$$

Let $0<\varepsilon<1/2$ be as in Hypothesis 8.3, that is,

$$(S-S_0)(S_0^2+I_{\mathcal{H}})^{-k-\varepsilon}\in\mathcal{B}_1(\mathcal{H}).$$

One estimates

$$\begin{aligned} &\big\|(S\pm i\theta I_{\mathcal{H}})^{-1}(S-S_0)(S_0\pm i\theta I_{\mathcal{H}})^{-1}(S_0^2+I_{\mathcal{H}})^{-k}\big\|_{\mathcal{B}_1(\mathcal{H})}\\ &\le\big\|(S\pm i\theta I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}(\mathcal{H})}\big\|(S-S_0)(S_0^2+I_{\mathcal{H}})^{-k-\varepsilon}\big\|_{\mathcal{B}_1(\mathcal{H})}\big\|(S_0^2+\theta^2 I_{\mathcal{H}})^{-1/2+\varepsilon}\big\|_{\mathcal{B}(\mathcal{H})}\\ &\le\theta^{-2+2\varepsilon}\big\|(S-S_0)(S_0^2+I_{\mathcal{H}})^{-k-\varepsilon}\big\|_{\mathcal{B}_1(\mathcal{H})},\end{aligned}$$

implying,

$$\begin{aligned} &\bigg\|\int_1^\infty\frac{\theta d\theta}{(\theta^2-1)^{1/2}}(S\pm i\theta I_{\mathcal{H}})^{-1}(S-S_0)(S_0\pm i\theta I_{\mathcal{H}})^{-1}(S_0^2+I_{\mathcal{H}})^{-k}\bigg\|_{\mathcal{B}_1(\mathcal{H})}\\ &\qquad\qquad\le\int_1^\infty\frac{d\theta}{(\theta^2-1)^{1/2}\theta^{1-2\varepsilon}}\big\|(S-S_0)(S_0^2+I_{\mathcal{H}})^{-k-\varepsilon}\big\|_{\mathcal{B}_1(\mathcal{H})}.\end{aligned}$$

Since $\varepsilon < 1/2$, it follows that $\int_1^\infty d\theta(\theta^2-1)^{-1/2}\theta^{2\varepsilon-1} < \infty$ and thus the integral

$$\int_1^\infty \frac{\theta d\theta}{(\theta^2-1)^{1/2}}(S \pm i\theta I_{\mathcal{H}})^{-1}(S-S_0)(S_0 \pm i\theta I_{\mathcal{H}})^{-1}(S_0^2+I_{\mathcal{H}})^{-k}$$

converges in $\mathcal{B}_1(\mathcal{H})$. ■

Lemma 8.11. *Assume Hypothesis 8.3 with $r = 2k$ for some $k \in \mathbb{N}$. For the function ϕ introduced in (8.12) one concludes that*

$$\big[\big(\phi(S)+iI_{\mathcal{H}}\big)^{-1} - \big(\phi(S_0)+iI_{\mathcal{H}}\big)^{-1}\big] \in \mathcal{B}_1(\mathcal{H}).$$

Proof. One writes

$$\begin{aligned}
\big[\phi(t)+i\big]^{-1} &= \big[t(1+t^2)^{k-(1/2)}+i\big]^{-1} \\
&= \frac{t(1+t^2)^{k-(1/2)}}{t^2(1+t^2)^{2k-1}+1} - i\frac{1}{t^2(1+t^2)^{2k-1}+1} \\
&= \frac{t}{(t^2+1)^{1/2}}\frac{(1+t^2)^k}{t^2(1+t^2)^{2k-1}+1} - i\frac{1}{t^2(1+t^2)^{2k-1}+1},
\end{aligned}$$

that is,

$$\big[\phi(t)+i\big]^{-1} = g(t)h_1(t) - ih_2(t), \quad t \in \mathbb{R},$$

where h_1, h_2 are introduced in Lemma 8.9 and g in Lemma 8.10. Therefore,

$$\begin{aligned}
&\big[\big(\phi(S)+iI_{\mathcal{H}}\big)^{-1} - \big(\phi(S_0)+iI_{\mathcal{H}}\big)^{-1}\big] \\
&= g(S)h_1(S) - g(S_0)h_1(S_0) - i\big[h_2(S)-h_2(S_0)\big] \\
&= \big[g(S)-g(S_0)\big]h_1(S_0) + g(S)\big[h_1(S)-h_1(S_0)\big] - i\big[h_2(S)-h_2(S_0)\big],
\end{aligned}$$

and by Lemma 8.10 one concludes that

$$\big[g(S)-g(S_0)\big]h_1(S_0) \in \mathcal{B}_1(\mathcal{H}).$$

Thus, Lemma 8.9 implies

$$h_j(S)-h_j(S_0) = f_j\big((S^2+I_{\mathcal{H}})^{-k}\big) - f_j\big((S_0^2+I_{\mathcal{H}})^{-k}\big), \quad j = 1,2,$$

with $f_j \in C^{1,\frac{1}{k}}([0,1])$, $j = 1,2$. Lemma 8.8 then yields

$$\big[(S^2+I_{\mathcal{H}})^{-k} - (S_0^2+I_{\mathcal{H}})^{-k}\big] \in \mathcal{B}_1(\mathcal{H}).$$

Thus, by Theorem 8.7 one obtains

$$\big[f_j\big((S^2+I_{\mathcal{H}})^{-k}\big) - f_j\big((S_0^2+I_{\mathcal{H}})^{-k}\big)\big] \in \mathcal{B}_1(\mathcal{H}), \quad j = 1,2,$$

and hence,

$$\big[\big(\phi(S)+iI_{\mathcal{H}}\big)^{-1} - \big(\phi(S_0)+iI_{\mathcal{H}}\big)^{-1}\big] \in \mathcal{B}_1(\mathcal{H}),$$

as required. ■

The following theorem improves the integrability condition in (8.5) for even $r \in \mathbb{N}$.

Theorem 8.12. *Assume Hypothesis 8.3 with $r = 2k$ for some $k \in \mathbb{N}$. For any $f \in \mathfrak{F}_r(\mathbb{R})$ one has*

$$\big[f(S) - f(S_0)\big] \in \mathcal{B}_1(\mathcal{H}),$$

and there exists a function

$$\xi(\,\cdot\,; S, S_0) \in L^1\big(\mathbb{R}; (1 + |\lambda|)^{-r-1}\, d\lambda\big) \tag{8.15}$$

such that the following trace formula holds,

$$\operatorname{tr}_{\mathcal{H}}\big(f(S) - f(S_0)\big) = \int_{\mathbb{R}} \xi(\lambda; S, S_0) d\lambda\, f'(\lambda), \quad f \in \mathfrak{F}_r(\mathbb{R}). \tag{8.16}$$

In particular, one has

$$\big[(S - zI_{\mathcal{H}})^{-r} - (S_0 - zI_{\mathcal{H}})^{-r}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{8.17}$$

and

$$\operatorname{tr}_{\mathcal{H}}\big((S - zI_{\mathcal{H}})^{-r} - (S_0 - zI_{\mathcal{H}})^{-r}\big) = -r\int_{\mathbb{R}} \frac{\xi(\lambda; S, S_0)d\lambda}{(\lambda - z)^{r+1}}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{8.18}$$

Proof. Let ϕ be as in (8.12). Then Lemma 8.11 implies that

$$\big[\big(\phi(S) + iI_{\mathcal{H}}\big)^{-1} - \big(\phi(S_0) + iI_{\mathcal{H}}\big)^{-1}\big] \in \mathcal{B}_1(\mathcal{H}),$$

and hence there exists the spectral shift function

$$\xi\big(\,\cdot\,; \phi(S), \phi(S_0)\big) \in L^1\big([0,1]; \big(1 + |\lambda|\big)^{-2} d\lambda\big)$$

for the pair $(\phi(S), \phi(S_0))$. Since

$$\phi'(t) = (1 + t^2)^{(r-3)/2}(1 + rt^2) \geq 1 > 0,$$

it follows that ϕ is strictly monotone increasing on $\mathbb{R}$. Hence, we introduce the spectral shift function $\xi(\,\cdot\,; S, S_0)$ by setting

$$\xi(\lambda; S, S_0) = \xi\big(\phi(\lambda); \phi(S), \phi(S_0)\big) \quad \text{for a.e. } \lambda \in \mathbb{R}.$$

Since $\xi(\,\cdot\,; \phi(S), \phi(S_0)) \in L^1([0,1]; (1 + |\lambda|)^{-2} d\lambda)$, the definition of ϕ implies that

$$\xi(\,\cdot\,; S, S_0) \in L^1\big(\mathbb{R}; \big(1 + |\lambda|\big)^{-r-1}\, d\lambda\big).$$

Next, let $f \in \mathfrak{F}_r(\mathbb{R})$. Then $f \circ \phi^{-1} \in \mathfrak{F}_1(\mathbb{R})$, and hence (8.3) implies

$$\begin{aligned}\operatorname{tr}_{\mathcal{H}}\big(f(S) - f(S_0)\big) &= \operatorname{tr}_{\mathcal{H}}\big((f \circ \phi^{-1})\big(\phi(S)\big) - (f \circ \phi^{-1})(\phi(S_0))\big)\\ &= \int_0^1 \xi\big(\mu; \phi(S), \phi(S_0)\big) d\mu \frac{f'\big(\phi^{-1}(\mu)\big)}{\phi'\big(\phi^{-1}(\mu)\big)}\end{aligned}$$

$$= \int_{\mathbb{R}} \xi\big(\phi(\lambda); \phi(S), \phi(S_0)\big) d\lambda \; f'(\lambda)$$

$$= \int_{\mathbb{R}} \xi(\lambda; S, S_0) d\lambda \; f'(\lambda),$$

proving (8.16).

Since for any $z \in \mathbb{C} \backslash \mathbb{R}$ the map $\lambda \mapsto (\lambda - z)^{-r}$, $\lambda \in \mathbb{R}$, belongs to the class $\mathfrak{F}_r(\mathbb{R})$, the trace formula (8.18) is a particular case of formula (8.16). ■