Chapter 9

Representing $\xi(\,\cdot\,; S, S_0)$ in terms of regularized Fredholm determinants

In this chapter, we establish the representation of $\xi(\,\cdot\,; S, S_0)$ in terms of regularized Fredholm determinants.

Hypothesis 9.1. *Let S_0 and S be self-adjoint operators in $\mathcal{H}$ with $(S - S_0) \in \mathcal{B}(\mathcal{H})$.*

(i) *If $r \in \mathbb{N}$ is odd, assume* (8.4)*, that is,*

$$\big[(S - zI_{\mathcal{H}})^{-r} - (S_0 - zI_{\mathcal{H}})^{-r}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{9.1}$$

and

$$(S - S_0)(S_0 - zI_{\mathcal{H}})^{-j} \in \mathcal{B}_{(r+1)/j}(\mathcal{H}), \quad j \in \mathbb{N},\ 1 \leq j \leq r + 1. \tag{9.2}$$

(ii) *If $r \in \mathbb{N}$ is even, assume the remaining conditions in Hypothesis* 8.3*, that is, for some $0 < \varepsilon < 1/2$,*

$$(S - S_0)(S_0^2 + I_{\mathcal{H}})^{-(r/2)-\varepsilon} \in \mathcal{B}_1(\mathcal{H}). \tag{9.3}$$

By Remark 8.4 (i), (9.2) holds for odd and even r.

Remark 9.2. In the applications to multidimensional Dirac operators to be considered in the sequel, the number r in (9.2) is the dimension of the underlying Euclidean space $\mathbb{R}^n$, that is, $r = n$, $n \in \mathbb{N}$, $n \geq 2$, as detailed in Lemma 7.2. ◇

By Theorem 8.5, Hypothesis 9.1 implies

$$\big[(S - zI_{\mathcal{H}})^{-r} - (S_0 - zI_{\mathcal{H}})^{-r}\big] \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{9.4}$$

for odd and even r.

By Theorem 8.12 the spectral shift function $\xi(\,\cdot\,; S, S_0)$ exists and (8.5) and (8.18) hold. The main aim of the present chapter is to obtain an almost everywhere representation for $\xi(\,\cdot\,; S, S_0)$ in terms of the regularized perturbation determinants of the operators $(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}$, $z \in \mathbb{C}\backslash\mathbb{R}$.

To set the stage, we begin by recalling some basic definitions and results pertaining to regularized determinants to be used in the sequel. For detailed discussions of regularized determinants, we refer to [159, Chapters 3, 5, and 9] and [184, Section 1.7].

Let $\{h_n\}_{n=1}^{\infty}$ denote an orthonormal basis for $\mathcal{H}$ and suppose $A \in \mathcal{B}_1(\mathcal{H})$. For each $N \in \mathbb{N}$, let $M_N \in \mathbb{C}^{N\times N}$ denote the matrix with entries

$$\delta_{j,k} + (h_j, Ah_k)_{\mathcal{H}}, \quad 1 \leq j,k \leq N.$$

The sequence $\{\det_{\mathbb{C}^{N\times N}}(M_N)\}_{N=1}^{\infty}$ has a limit as $N \to \infty$, and its value does not depend on the orthonormal basis chosen. One defines the Fredholm determinant

$$\det_{\mathcal{H}}(I_{\mathcal{H}} + A) := \lim_{N\to\infty} \det_{\mathbb{C}^{N\times N}}(M_N).$$

The Fredholm determinant is continuous with respect to $\|\cdot\|_{\mathcal{B}_1(\mathcal{H})}$. That is, if $\{A_n\}_{n=1}^{\infty} \subset \mathcal{B}_1(\mathcal{H})$ and $\lim_{n\to\infty} \|A_n - A\|_{\mathcal{B}_1(\mathcal{H})} = 0$, then

$$\lim_{n\to\infty} \det_{\mathcal{H}}(I_{\mathcal{H}} + A_n) = \det_{\mathcal{H}}(I_{\mathcal{H}} + A). \tag{9.5}$$

In fact, the Fredholm determinant is Fréchet differentiable with respect to A (cf., e.g., [159, Theorem 5.2]). Moreover, if $\Omega \subseteq \mathbb{C}$ is an open set and $A : \Omega \to \mathcal{B}_1(\mathcal{H})$ is analytic, then the function $\det_{\mathcal{H}}(I_{\mathcal{H}} + A(\cdot))$ is analytic in Ω, and

$$\frac{d}{dz} \log\big(\det_{\mathcal{H}}\big(I_{\mathcal{H}} + A(z)\big)\big) = \operatorname{tr}_{\mathcal{H}}\Big(\big(I_{\mathcal{H}} + A(z)\big)^{-1} A'(z)\Big).$$

The definition of the Fredholm determinant given in (9.5) is generally not meaningful if $A \in \mathcal{B}_p(\mathcal{H})$ with $p \in \mathbb{N}\backslash\{1\}$. To give meaning to the determinant in this case, suitable modifications are needed. For $p \in \mathbb{N}\backslash\{1\}$, one introduces the function $R_p : \mathcal{B}_p(\mathcal{H}) \to \mathcal{B}_1(\mathcal{H})$ by

$$R_p(A) = (I_{\mathcal{H}} + A)e^{\sum_{j=1}^{p-1}(-1)^j j^{-1} A^j} - I_{\mathcal{H}}, \quad A \in \mathcal{B}_p(\mathcal{H}). \tag{9.6}$$

Then the regularized (or modified) Fredholm determinant is defined by

$$\det_{\mathcal{H},p}(I_{\mathcal{H}} + A) = \det_{\mathcal{H}}\big(I_{\mathcal{H}} + R_p(A)\big), \quad A \in \mathcal{B}_p(\mathcal{H}), \quad p \in \mathbb{N}\backslash\{1\}. \tag{9.7}$$

The Fredholm determinant $\det_{\mathcal{H},p}(\cdot)$ retains many of the properties of the ordinary Fredholm determinant. For example, $\det_{\mathcal{H},p}(I_{\mathcal{H}} + A)$ is continuous with respect to $A \in \mathcal{B}_p(\mathcal{H})$: if $A \in \mathcal{B}_p(\mathcal{H})$, $\{A_n\}_{n=1}^{\infty} \subset \mathcal{B}_p(\mathcal{H})$, and $\lim_{n\to\infty} \|A_n - A\|_{\mathcal{B}_p(\mathcal{H})} = 0$, then

$$\lim_{n\to\infty} \det_{\mathcal{H},p}(I_{\mathcal{H}} + A_n) = \det_{\mathcal{H},p}(I_{\mathcal{H}} + A).$$

In addition, if $\Omega \subseteq \mathbb{C}$ is open and $A : \Omega \to \mathcal{B}_p(\mathcal{H})$ is analytic in Ω, then the function $\det_{\mathcal{H},p}(I_{\mathcal{H}} + A(\cdot))$ is analytic in Ω and

$$\begin{aligned} &\frac{d}{dz} \log\big(\det_{\mathcal{H},p}\big(I_{\mathcal{H}} + A(z)\big)\big) \\ &\quad = (-1)^{p-1} \operatorname{tr}_{\mathcal{H}}\Big(\big(I_{\mathcal{H}} + A(z)\big)^{-1} A^{p-1}(z) A'(z)\Big). \end{aligned} \tag{9.8}$$

The importance of the regularized determinant stems from the fact that for $A \in \mathcal{B}_p(\mathcal{H})$, the operator $I_{\mathcal{H}} + A$ is boundedly invertible (i.e., $-1 \in \rho(A)$) if and only if $\det_{\mathcal{H},p}(I_{\mathcal{H}} + A) \neq 0$ (cf., e.g., [159, Theorem 9.2]). Equivalently, $-1 \in \sigma(A)$ if and only if $\det_{\mathcal{H},p}(I_{\mathcal{H}} + A) = 0$.

Finally, we note the cyclicity property of the regularized determinant: if $A, B \in \mathcal{B}(\mathcal{H})$ are such that $AB, BA \in \mathcal{B}_p(\mathcal{H})$, then

$$\det_{\mathcal{H},p}(I_{\mathcal{H}} + AB) = \det_{\mathcal{H},p}(I_{\mathcal{H}} + BA). \tag{9.9}$$

In particular, if $A \in \mathcal{B}_p(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$, then (9.9) holds. Similarly, if $A, B \in \mathcal{B}(\mathcal{H})$ are such that $AB, BA \in \mathcal{B}_1(\mathcal{H})$, then

$$\operatorname{tr}_{\mathcal{H}}(AB) = \operatorname{tr}_{\mathcal{H}}(BA). \tag{9.10}$$

With these preliminaries in hand, we start with introducing the regularized determinant associated with the (non-symmetrized) Birman–Schwinger-type operator

$$B(z) := (S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{9.11}$$

Lemma 9.3. *Assume Hypothesis 9.1. The map*

$$B(z) = (S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{9.12}$$

is a $\mathcal{B}_{r+1}(\mathcal{H})$-valued analytic function.

Proof. Let $z_0 \in \mathbb{C}\backslash\mathbb{R}$ be fixed. Then (see e.g. [183, Theorem 5.14])

$$(S_0 - zI_{\mathcal{H}})^{-1} = \sum_{k=0}^{\infty} (S_0 - z_0 I_{\mathcal{H}})^{-k-1}(z - z_0)^k,$$

where the series converges with respect to the $\mathcal{B}(\mathcal{H})$-norm for all $z \in \mathbb{C}\backslash\mathbb{R}$ such that $|z - z_0| < \|(S_0 - z_0 I_{\mathcal{H}})^{-1}\|_{\mathcal{B}(\mathcal{H})}^{-1} \leq |\operatorname{Im}(z_0)|^{-1}$. Therefore,

$$(S - S_0)(S_0 - zI_{\mathcal{H}})^{-1} = \sum_{k=0}^{\infty} (S - S_0)(S_0 - z_0 I_{\mathcal{H}})^{-k-1}(z - z_0)^k.$$

We claim that the latter series converges in the ball $\{z \in \mathbb{C} \mid |z - z_0| < |\operatorname{Im}(z_0)|\}$ in the $\mathcal{B}_{r+1}(\mathcal{H})$ norm. By (9.2), the operator

$$B(z) = (S - S_0)(S_0 - z_0 I_{\mathcal{H}})^{-1} \in \mathcal{B}_{r+1}(\mathcal{H}),$$

so that

$$\begin{aligned}
&\big\|(S - S_0)(S_0 - z_0 I_{\mathcal{H}})^{-k-1}\big\|_{\mathcal{B}_{r+1}(\mathcal{H})} \\
&\quad \leq \big\|(S - S_0)(S_0 - z_0 I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}_{r+1}(\mathcal{H})} \big\|(S_0 - z_0 I_{\mathcal{H}})^{-k}\big\|_{\mathcal{B}(\mathcal{H})} \\
&\quad \leq \big\|(S - S_0)(S_0 - z_0 I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}_{r+1}(\mathcal{H})} \big|\operatorname{Im}(z_0)\big|^{-k}.
\end{aligned}$$

This proves the convergence. ∎

Lemma 9.4. *Assume Hypothesis 9.1. The function*

$$F_{S,S_0}(z) := \ln\big(\det_{\mathcal{H},r+1}\big((S - zI_{\mathcal{H}})(S_0 - zI_{\mathcal{H}})^{-1}\big)\big), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{9.13}$$

is well-defined, in fact, analytic in $\mathbb{C}\backslash\mathbb{R}$.

Proof. By the second resolvent identity,

$$(S - zI_{\mathcal{H}})(S_0 - zI_{\mathcal{H}})^{-1} = I_{\mathcal{H}} + B(z), \quad z \in \mathbb{C}\backslash\mathbb{R},$$

where $B(\cdot)$ is the $\mathcal{B}_{r+1}(\mathcal{H})$-valued analytic function defined in (9.12). Hence, by the properties of regularized determinants the function

$$z \to \det_{\mathcal{H},r+1}\big(I_{\mathcal{H}} + B(z)\big)$$

is analytic in $\mathbb{C}_{\pm}$. Combining the Cauchy integral theorem and [128, Theorem V.4.1], one infers that the function

$$z \to \ln\big(\det_{\mathcal{H},r+1}\big(I_{\mathcal{H}} + B(z)\big)\big)$$

is a well-defined analytic function in $\mathbb{C}_{\pm}$, provided that $\det_{\mathcal{H},r+1}(I_{\mathcal{H}} + B(z)) \neq 0$ for all $z \in \mathbb{C}\backslash\mathbb{R}$. Thus, it remains to show, that $\det_{\mathcal{H},r+1}(I_{\mathcal{H}} + B(z)) \neq 0$ for every $z \in \mathbb{C}\backslash\mathbb{R}$. If $\det_{\mathcal{H},r+1}(I_{\mathcal{H}} + B(z)) = 0$ for some $z \in \mathbb{C}\backslash\mathbb{R}$, then -1 is in the spectrum of $B(z)$. By compactness of $B(\cdot)$, -1 is an eigenvalue of $B(z)$, and therefore, $I_{\mathcal{H}} + B(z)$ has a nontrivial kernel. Since S_0 is self-adjoint and hence $z \in \mathbb{C}\backslash\mathbb{R}$ cannot be an eigenvalue of S_0, z is an eigenvalue for S, which, once more, cannot be the case since S is also self-adjoint. ■

To correlate the function $\ln(\det_{\mathcal{H},r+1}(I_{\mathcal{H}} + B(\cdot)))$ with the spectral shift function for the pair (S, S_0), we need to introduce an auxiliary function.

Lemma 9.5. *Assume Hypothesis 9.1 and let $B(\cdot)$ be defined by (9.12). There exists an analytic function $G_{S,S_0}(\cdot)$ in $\mathbb{C}\backslash\mathbb{R}$ such that*

$$\begin{aligned}\frac{d^r}{dz^r} G_{S,S_0}(z) \\ &= \operatorname{tr}_{\mathcal{H}}\bigg(\frac{d^{r-1}}{dz^{r-1}}\sum_{j=0}^{r-1}(-1)^{r-j}(S_0 - zI_{\mathcal{H}})^{-1}B(z)^{r-j}\bigg), \quad z \in \mathbb{C}\backslash\mathbb{R}.\end{aligned} \tag{9.14}$$

Proof. It suffices to prove that each of the terms

$$\operatorname{tr}_{\mathcal{H}}\bigg(\frac{d^{r-1}}{dz^{r-1}}(S_0 - zI_{\mathcal{H}})^{-1}B(z)^{r-j}\bigg), \quad z \in \mathbb{C}\backslash\mathbb{R},\ j \in \mathbb{N}_0,\ 0 \leq j \leq r-1, \tag{9.15}$$

defines an analytic function. To analyze the operator under the trace in (9.15), we introduce multi-indices. Recalling $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$, for $\nu \in \mathbb{N}$ an element $\underline{k} \in \mathbb{N}_0^{\nu}$ is called a multi-index which we express componentwise as

$$\underline{k} = (k_1, \dots, k_\nu) \in \mathbb{N}_0^\nu, \quad k_p \in \mathbb{N}_0,\ 1 \le p \le \nu. \tag{9.16}$$

The order of the multi-index $\underline{k} \in \mathbb{N}_0^\nu$ is defined to be

$$|\underline{k}| := k_1 + \cdots + k_\nu. \tag{9.17}$$

For each fixed $j \in \mathbb{N}_0$ with $0 \le j \le r-1$,

$$\begin{aligned}&\frac{d^{r-1}}{dz^{r-1}}(S_0 - zI_{\mathcal{H}})^{-1}B(z)^{r-j}\\ &\quad = \sum_{\substack{\underline{k}\in\mathbb{N}_0^{r-j+1}\\ |\underline{k}|=r-1}} c_{j,\underline{k}}(S_0 - zI_{\mathcal{H}})^{-(k_1+1)} \prod_{\ell=2}^{r-j+1} (S - S_0)(S_0 - I_{\mathcal{H}})^{-(k_\ell+1)},\end{aligned} \tag{9.18}$$

for an appropriate set of z-independent scalars

$$c_{j,\underline{k}} \in \mathbb{R}, \quad \underline{k} \in \mathbb{N}_0^{r-j+1},\ |\underline{k}| = r-1.$$

The assumption (9.2) and the analog of Hölder's inequality for trace ideals (see [159, Theorem 2.8]) imply that each term in the sum in (9.18) is a trace class operator. In particular, (9.18) implies that the operator $\frac{d^{r-1}}{dz^{r-1}}(S_0 - zI_{\mathcal{H}})^{-1}B(z)^{r-j}$ is a trace class operator. Repeating the argument in Lemma 9.3 and employing (9.2), one concludes that the map

$$\mathbb{C}\backslash\mathbb{R} \ni z \to \frac{d^{r-1}}{dz^{r-1}}(S_0 - zI_{\mathcal{H}})^{-1}B(z)^{r-j}, \quad 0 \le j \le r-1,$$

is a $\mathcal{B}_1(\mathcal{H})$-valued analytic function. ■

The following lemma is the main result, which allows to correlate the regularized determinant of the operator $I_{\mathcal{H}} + (S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}$ and the spectral shift function $\xi(\,\cdot\,, S, S_0)$ (see Theorem 9.9 below).

Lemma 9.6. *Assume Hypothesis 9.1. If F_{S,S_0} and G_{S,S_0} denote the analytic functions in $\mathbb{C}\backslash\mathbb{R}$ introduced in (9.13) and (9.14), respectively, then there exist polynomials $P_{\pm,r-1}$ of degree less than or equal to $r-1$ such that*

$$F_{S,S_0}(z) = (z-i)^r \int_{\mathbb{R}} \frac{\xi(\lambda; S, S_0)\,d\lambda}{(\lambda - i)^r}\,\frac{1}{\lambda - z} + G_{S,S_0}(z) + P_{\pm,r-1}(z), \quad z \in \mathbb{C}_\pm.$$

Proof. One recalls the $\mathcal{B}_{r+1}(\mathcal{H})$-valued analytic function $B(\cdot)$ defined in (9.12). By the second resolvent identity,

$$\big(I_{\mathcal{H}} + B(z)\big)^{-1} = \big(I_{\mathcal{H}} + (S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}\big)^{-1}$$

$$
\begin{aligned}
&= \big((S - zI_{\mathcal{H}})(S_0 - zI_{\mathcal{H}})^{-1}\big)^{-1} \\
&= (S_0 - zI_{\mathcal{H}})(S - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned}
$$

In addition,

$$B'(z) = B(z)(S_0 - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}.$$

Applying (9.8), one obtains

$$
\begin{aligned}
&\frac{d}{dz} F_{S,S_0}(z) \\
&= \frac{d}{dz} \ln\big(\det{}_{\mathcal{H},r+1}(I_{\mathcal{H}} + B(z))\big) \\
&= (-1)^m \operatorname{tr}_{\mathcal{H}}\big((S_0 - zI_{\mathcal{H}})(S - zI_{\mathcal{H}})^{-1} B(z)^r B(z)(S_0 - zI_{\mathcal{H}})^{-1}\big) \\
&= (-1)^m \operatorname{tr}_{\mathcal{H}}\big((S_0 - zI_{\mathcal{H}})(S - zI_{\mathcal{H}})^{-1} B(z)^{r+1}(S_0 - zI_{\mathcal{H}})^{-1}\big), \quad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned}
$$

For $z \in \mathbb{C}\backslash\mathbb{R}$, $(S_0 - zI_{\mathcal{H}})(S - zI_{\mathcal{H}})^{-1} \in \mathcal{B}(\mathcal{H})$ and $B(z)^{r+1} \in \mathcal{B}_1(\mathcal{H})$ (cf. (9.2)), so that

$$
\begin{aligned}
\frac{d}{dz} F_{S,S_0}(z) &= (-1)^r \operatorname{tr}_{\mathcal{H}}\big(B(z)^{r+1}(S_0 - zI_{\mathcal{H}})^{-1}(S_0 - zI_{\mathcal{H}})(S - zI_{\mathcal{H}})^{-1}\big) \\
&= (-1)^r \operatorname{tr}_{\mathcal{H}}\big(B(z)^{r+1}(S - zI_{\mathcal{H}})^{-1}\big) \\
&= (-1)^r \operatorname{tr}_{\mathcal{H}}\big((S - zI_{\mathcal{H}})^{-1} B(z)^{r+1}\big), \quad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{9.19}
$$

By the second resolvent identity,

$$
\begin{aligned}
(S - z)^{-1} B(z) &= (S - z)^{-1}(S - S_0)(S_0 - z)^{-1} \\
&= (S_0 - z)^{-1} - (S - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned} \tag{9.20}
$$

and repeated application of (9.20) yields

$$
\begin{aligned}
&(-1)^r (S - zI_{\mathcal{H}})^{-1} B(z)^{r+1} \\
&\quad = (-1)^r \big((S_0 - zI_{\mathcal{H}})^{-1} - (S - zI_{\mathcal{H}})^{-1}\big) B(z)^r \\
&\quad = (S_0 - zI_{\mathcal{H}})^{-1} \sum_{j=0}^{r-1} (-1)^{r-j} B(z)^{r-j} \\
&\qquad + (S_0 - zI_{\mathcal{H}})^{-1} - (S - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{9.21}
$$

Hence, combining (9.19) with (9.21), one obtains

$$
\begin{aligned}
&\frac{d}{dz} F_{S,S_0}(z) \\
&= \operatorname{tr}_{\mathcal{H}}\left((S_0 - zI_{\mathcal{H}})^{-1} - (S - zI_{\mathcal{H}})^{-1} + (S_0 - zI_{\mathcal{H}})^{-1} \sum_{j=0}^{r-1} (-1)^{r-j} B(z)^{r-j}\right), \\
&\hspace{20em} z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{9.22}
$$

Differentiating (9.22) $r-1$ times,

$$\begin{aligned}
&\frac{d^r}{dz^r} F_{S,S_0}(z) \\
&\quad = \frac{d^{r-1}}{dz^{r-1}} \operatorname{tr}_{\mathcal{H}} \bigg((S_0 - zI_{\mathcal{H}})^{-1} - (S - zI_{\mathcal{H}})^{-1} \\
&\qquad\qquad + (S_0 - zI_{\mathcal{H}})^{-1} \sum_{j=0}^{r-1} (-1)^{r-j} B(z)^{r-j} \bigg) \\
&\quad = \operatorname{tr}_{\mathcal{H}} \bigg((r-1)! \big((S_0 - zI_{\mathcal{H}})^{-r} - (S - zI_{\mathcal{H}})^{-r} \big) \\
&\qquad\qquad + \frac{d^{r-1}}{dz^{r-1}} (S_0 - zI_{\mathcal{H}})^{-1} \sum_{j=0}^{r-1} (-1)^{r-j} B(z)^{r-j} \bigg), \quad z \in \mathbb{C}\backslash\mathbb{R}. \qquad (9.23)
\end{aligned}$$

By (9.4) and Lemma 9.5, (9.23) may be recast as

$$\begin{aligned}
\frac{d^r}{dz^r} F_{S,S_0}(z) &= (r-1)! \operatorname{tr}_{\mathcal{H}} \big((S_0 - zI_{\mathcal{H}})^{-r} - (S - zI_{\mathcal{H}})^{-r} \big) \\
&\quad + \frac{d^r}{dz^r} G_{S,S_0}(z), \quad z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned}$$

and an application of Theorem 8.12 yields

$$\frac{d^r}{dz^r} F_{S,S_0}(z) = r! \int_{\mathbb{R}} \frac{\xi(\lambda; S, S_0)\, d\lambda}{(\lambda - z)^{r+1}} + \frac{d^r}{dz^r} G_{S,S_0}(z), \quad z \in \mathbb{C}\backslash\mathbb{R}. \qquad (9.24)$$

Repeated application of the elementary identity

$$\frac{k!}{(\lambda - z)^{k+1}} = \frac{d}{dz} \bigg(\frac{(k-1)!}{(\lambda - z)^k} - \frac{1}{(\lambda - i)^k} \bigg), \quad z \in \mathbb{C}\backslash\mathbb{R},\ \lambda \in \mathbb{R},\ k \in \mathbb{N},$$

yields

$$\begin{aligned}
\frac{r!}{(\lambda - z)^{r+1}} &= \frac{d^r}{dz^r} \bigg(\frac{1}{\lambda - z} - \sum_{j=1}^{r} \frac{(z-i)^{j-1}}{(\lambda - i)^j} \bigg) \\
&= \frac{d^r}{dz^r} \bigg(\frac{1}{\lambda - z} - \frac{(z-i)^r - (\lambda - i)^r}{(z - \lambda)(\lambda - i)^r} \bigg) \\
&= \frac{d^r}{dz^r} \bigg(\frac{(z-i)^r}{(\lambda - z)(\lambda - i)^r} \bigg), \quad z \in \mathbb{C}\backslash\mathbb{R},\ \lambda \in \mathbb{R}. \qquad (9.25)
\end{aligned}$$

Therefore, (9.24) and (9.25) imply

$$\begin{aligned}
&\frac{d^r}{dz^r} F_{S,S_0}(z) \\
&\quad = \frac{d^r}{dz^r} \int_{\mathbb{R}} \frac{\xi(\lambda; S, S_0) d\lambda\, (z-i)^r}{(\lambda - i)^r (\lambda - z)} + \frac{d^r}{dz^r} G_{S,S_0}(z), \quad z \in \mathbb{C}\backslash\mathbb{R},
\end{aligned}$$

completing the proof. ∎

Remark 9.7. For bookkeeping purposes we have thus far worked with the non-symmetrized Birman–Schwinger-type operator $B(z) := (S - S_0)(S_0 - zI_{\mathcal{H}})^{-1}$, $z \in \mathbb{C}\backslash\mathbb{R}$ and avoided a factorization of $S - S_0$ (and similarly we exploited V without its factorization (3.20) in Chapter 7). In the concrete case of massless Dirac operators H_0, H we will eventually switch over to a symmetrized analog (cf. (2.6)–(2.10), (10.78)). ◇

The main result of this chapter provides a means for recovering the spectral shift function $\xi(\,\cdot\,; S, S_0)$ almost everywhere in terms of the normal (or nontangential) boundary values of the functions $F_{S,S_0}(\,\cdot\,)$ and $G_{S,S_0}(\,\cdot\,)$ when the latter exist. Its proof relies on the following (special case of) Privalov's theorem (see, e.g., [184, Theorem 1.2.5]).

Theorem 9.8. *Let $\theta \in L^1\big(\mathbb{R}; (1 + |\lambda|)^{-1}\, d\lambda\big)$. If*

$$H(z) := \int_{\mathbb{R}} \frac{\theta(\lambda) d\lambda}{\lambda - z}, \quad z \in \mathbb{C}\backslash\mathbb{R},$$

then

$$\lim_{\varepsilon \downarrow 0} H(\lambda \pm i\varepsilon) = \pm\pi i \theta(\lambda) + \text{p.v.} \int_{\mathbb{R}} \frac{\theta(\lambda') d\lambda'}{\lambda' - \lambda} \quad \textit{for a.e. } \lambda \in \mathbb{R}, \tag{9.26}$$

where p.v.$(\,\cdot\,)$ *abbreviates the principal value operation. In particular, one obtains the following special case of the Stieltjes inversion theorem,*

$$\theta(\lambda) = (2\pi i)^{-1} \lim_{\varepsilon \downarrow 0} \big[H(\lambda + i\varepsilon) - H(\lambda - i\varepsilon)\big] \quad \textit{for a.e. } \lambda \in \mathbb{R}. \tag{9.27}$$

Moreover, the normal limits in (9.26) and (9.27) can be replaced by nontangential limits.

Theorem 9.9. *Assume Hypothesis 9.1 and let F_{S,S_0} and G_{S,S_0} denote analytic functions in $\mathbb{C}\backslash\mathbb{R}$ satisfying (9.13) and (9.14), respectively. If F_{S,S_0} and G_{S,S_0} have normal boundary values on $\mathbb{R}$, then for a.e. $\lambda \in \mathbb{R}$,*

$$\begin{aligned} \xi(\lambda; S, S_0) = \pi^{-1} \operatorname{Im}\big(F_{S,S_0}(\lambda + i0)\big) - \pi^{-1} \operatorname{Im}\big(G_{S,S_0}(\lambda + i0)\big) \\ + P_{r-1}(\lambda) \quad \textit{for a.e. } \lambda \in \mathbb{R}, \end{aligned} \tag{9.28}$$

where P_{r-1} is a polynomial of degree less than or equal to $r - 1$.

Proof. By Lemma 9.6,

$$\begin{aligned} F_{S,S_0}(z) = (z - i)^r \int_{\mathbb{R}} \frac{\xi(\lambda; S, S_0) d\lambda}{(\lambda - z)(\lambda - i)^r} + G_{S,S_0}(z) \\ + P_{\pm,r-1}(z), \quad z \in \mathbb{C}_{\pm}. \end{aligned} \tag{9.29}$$

If

$$H_{\pm}(z) := F_{S,S_0}(z) - G_{S,S_0}(z) - P_{\pm,r-1}(z), \quad z \in \mathbb{C}_{\pm},$$

then (9.29) may be recast as

$$\frac{H_{\pm}(z)}{(z-i)^r} = \int_{\mathbb{R}} \frac{\xi(\lambda; S, S_0)\,d\lambda}{(\lambda - z)(\lambda - i)^r}, \quad z \in \mathbb{C}_{\pm},\ z \neq i.$$

By (8.5), the spectral shift function $\xi(\cdot\,; S, S_0)$ satisfies

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

An application of Theorem 9.8 then yields

$$\begin{aligned}&\frac{\xi(\lambda; S, S_0)}{(\lambda - i)^r}\\ &\quad = (2\pi i)^{-1} \lim_{\varepsilon \downarrow 0} \left[\frac{H_+(\lambda + i\varepsilon)}{(\lambda + i\varepsilon - i)^r} - \frac{H_-(\lambda - i\varepsilon)}{(\lambda - i\varepsilon - i)^r}\right] \quad \text{for a.e. } \lambda \in \mathbb{R},\end{aligned}$$

and hence,

$$\xi(\lambda; S, S_0) = (2\pi i)^{-1} \lim_{\varepsilon \downarrow 0} \big[H_+(\lambda - i\varepsilon) - H_-(\lambda + i\varepsilon)\big] \quad \text{for a.e. } \lambda \in \mathbb{R}. \tag{9.30}$$

It follows from the definition of the functions F_{S,S_0} and G_{S,S_0} (cf. Lemmas 9.4 and 9.5) that

$$F_{S,S_0}(\bar{z}) = \overline{F_{S,S_0}(z)}, \quad G_{S,S_0}(\bar{z}) = \overline{G_{S,S_0}(z)}, \quad z \in \mathbb{C}\backslash\mathbb{R}.$$

Thus, by (9.30),

$$\begin{aligned}\xi(\lambda; S, S_0) &= (2\pi i)^{-1} \lim_{\varepsilon \downarrow 0} \big[F_{S,S_0}(\lambda + i\varepsilon) - F_{S,S_0}(\lambda - i\varepsilon)\big]\\ &\quad - (2\pi i)^{-1} \lim_{\varepsilon \downarrow 0} \big[G_{S,S_0}(\lambda + i\varepsilon) + G_{S,S_0}(\lambda - i\varepsilon)\big]\\ &\quad - (2\pi i)^{-1} \big[P_{+,r-1}(\lambda) - P_{-,r-1}(\lambda)\big]\\ &= \pi^{-1}\,\mathrm{Im}\big(F_{S,S_0}(\lambda + i0)\big) - \pi^{-1}\,\mathrm{Im}\big(G_{S,S_0}(\lambda + i0)\big)\\ &\quad + P_{r-1}(\lambda) \quad \text{for a.e. } \lambda \in \mathbb{R},\end{aligned}$$

where the polynomial $P_{r-1} := (2\pi i)^{-1}[P_{-,r-1} - P_{+,r-1}]$ has degree less than or equal to $r-1$ (since $P_{\pm,r-1}$ have degree less than or equal to $r-1$). ■